

Second order semiclassics with self-generated magnetic fields

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Abstract

We consider the semiclassical asymptotics of the sum of negative eigenvalues of the three-dimensional Pauli operator with an external potential and a self-generated magnetic field B . We also add the field energy $\beta \int B^2$ and we minimize over all magnetic fields. The parameter β effectively determines the strength of the field. We consider the weak field regime with $\beta h^2 \geq \text{const} > 0$, where h is the semiclassical parameter. For smooth potentials we prove that the semiclassical asymptotics of the total energy is given by the non-magnetic Weyl term to leading order with an error bound that is smaller by a factor $h^{1+\varepsilon}$, i.e. the subleading term vanishes. However, for potentials with a Coulomb singularity the subleading term does not vanish due to the non-semiclassical effect of the singularity. Combined with a multiscale technique, this refined estimate is

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used in the companion paper [EFS3] to prove the second order Scott correction to the ground state energy of large atoms and molecules.

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1 Introduction

An important problem in semiclassical spectral analysis is to determine the sum of the negative eigenvalues of a Schrödinger operator $-h^2\Delta - V(x)$ on $L^2(\mathbb{R}^d)$, i.e.,

$$\mathrm{Tr} (-h^2\Delta - V(x))_-.$$

We will use the convention that $x_- = (x)_- = \min\{x, 0\}$ when x is either a real number or a self-adjoint operator. It is well known that under appropriate integrability conditions on V the leading order term is given by the Weyl asymptotics

$$\mathrm{Tr} (-h^2\Delta - V(x))_- = (2\pi h)^{-d} \iint_{\mathbb{R}^d \times \mathbb{R}^d} (p^2 - V(x))_- dx dp + o(h^{-d}), \quad h \rightarrow 0, \quad (1.1)$$

and for smooth potentials the error term can be improved to $O(h^{-d+2})$ (under some non-criticality assumption) by using pseudo-differential calculus. In other words, the subleading term in the semiclassical expansion in powers of h vanishes. We remark that with more elementary methods and under less regularity assumptions on V , for a local version of this problem

$$\mathrm{Tr} [\psi(-h^2\Delta - V(x))\psi]_-, \quad \psi \in C_0^\infty(\mathbb{R}^d),$$

the error term has been shown to be $O(h^{-d+6/5})$ in Theorem 12 of [SS] (we will recall it in Theorem 3.3). This bound was extended to the relativistic case in [SSS].

A generalization of this problem is to consider not only a potential V but also an exterior magnetic field $B = \nabla \times A$ generated by a vector potential A . The corresponding magnetic Schrödinger operator is $(-i\nabla + A)^2 - V(x)$. A further generalization is to consider the particles as having spin $-\frac{1}{2}$ and introduce the magnetic Pauli operator $[\boldsymbol{\sigma} \cdot (-i\nabla + A)]^2 - V$, where in $d = 3$ dimensions $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ denotes the vector of Pauli matrices. For simplicity we will consider the $d = 3$ dimensional case only and we denote both the Schrödinger operator $(-ih\nabla + A)^2$ and the Pauli operator $[\boldsymbol{\sigma} \cdot (-ih\nabla + A)]^2$ by $T_h(A)$. Our analysis will be carried out in the more complicated case of the Pauli operator, analogous but easier results can be proved for the Schrödinger case as well.

Much work has gone into understanding the semiclassical asymptotics of the sum of negative eigenvalues, i.e., the asymptotics for small $h > 0$ of

$$\text{Tr} (T_h(A) - V(x))_-.$$

It is well known that under appropriate conditions on A and V the leading behavior as h tends to zero is given by the Weyl asymptotics (1.1) and note that the limit behavior is non-magnetic, i.e. fixed magnetic fields do not influence the leading order semiclassics. If the magnetic field is rescaled, $B \rightarrow \mu B$, and the coupling constant μ increases along with the $h \rightarrow 0$ semiclassical limit at least as $\mu \gtrsim h^{-1}$, then magnetic fields become relevant even in the leading term. Most work in this direction has been carried out with a homogeneous magnetic field [Sob, LSY1, LSY2] with some generalization to an inhomogeneous one [ES, I] but always subject to regularity conditions on the field.

In this paper we will address a related and equally important issue, namely the case when the magnetic field is not a fixed external field, but the self-generated classical magnetic field generated by the particles themselves. The vector potential A will be optimized to minimize the total energy consisting of the sum of negative eigenvalues (corresponding to the ground state energy of non-interacting fermions) and the field energy

$$\int B^2 = \int |\nabla \times A|^2$$

(we use the convention that unspecified integrals are always on \mathbb{R}^3 w.r.t. the Lebesgue measure). The problem we consider is thus to determine the energy

$$E(\beta, h, V) = \inf_A \left[\text{Tr} (T_h(A) - V)_- + \beta \int |\nabla \times A|^2 \right] \quad (1.2)$$

for $\beta, h > 0$, where the infimum runs over all vector fields $A \in H^1(\mathbb{R}^3; \mathbb{R}^3)$; in fact minimizing only for all $A \in C_0^\infty(\mathbb{R}^3; \mathbb{R}^3)$ gives the same infimum. Alternatively, in addition to $A \in H^1(\mathbb{R}^3; \mathbb{R}^3)$, one could impose a gauge fixing condition, e.g., $\nabla \cdot A = 0$, see more details in Appendix A of [EFS1].

Here β is an additional parameter setting the strength of the coupling of the particles to the field. Formally $\beta = \infty$ corresponds to the non-magnetic case; smaller β means that a larger optimizing magnetic field is expected. In a given physical system the values of h and β are given, but as is standard in semiclassical analysis we leave them as free parameters.

The Euler-Lagrange equation corresponding to the variational problem (1.2) above is

$$\beta \nabla \times B = J_A, \quad (1.3)$$

where J_A is the current of the Fermi gas, which in the Schrödinger case is

$$J_A(x) = -\text{Re} \left[(-ih\nabla + A) 1_{(-\infty, 0]}(T_h(A) - V) \right] (x, x)$$

and in the Pauli case is

$$J_A(x) = -\text{Re} \left[\text{Tr}_{\mathbb{C}^2} \left(\boldsymbol{\sigma}(\boldsymbol{\sigma} \cdot (-ih\nabla + A)) 1_{(-\infty, 0]}(T_h(A) - V) \right) \right] (x, x).$$

In other words the Euler-Lagrange equations are the non-linear coupled Maxwell-Schrödinger or Maxwell-Pauli equations.

Semiclassical results with magnetic fields mentioned above assume that the field is regular. However, if the magnetic field arises as self-generated and thus determined internally via a variational principle, the sufficient regularity is not a-priori given.

The first semiclassical result for the local problem with a self-generated magnetic field was presented in [ES3], where the leading order asymptotics was shown to be given by the non-magnetic Weyl term in the weak field regime, $\beta h^2 \geq \text{const} > 0$. The error term was by a factor of order $h^{1/2}$ smaller than the leading term (see Theorem 1.3 of [ES] for the lower bound; the matching upper bound was not explicitly stated in [ES] but it clearly follows by choosing $A \equiv 0$).

The main result of this paper is a substantial improvement of the error term to a factor of order $h^{1+\varepsilon}$. This result can also be interpreted as showing that the subleading term in the semiclassical expansion in powers of h vanishes.

Theorem 1.1. *Let $V \in C_0^\infty(\mathbb{R}^3)$. There exist a universal constant $\varepsilon > 0$ such that for any fixed $\kappa_0 > 0$ we have*

$$\lim_{h \rightarrow 0, \beta h^2 \geq \kappa_0} h^{2-\varepsilon} \left| E(\beta, h, V) - 2(2\pi h)^{-3} \iint [p^2 - V(q)]_- dp dq \right| = 0 \quad (1.4)$$

for the Pauli problem. The same result (without the prefactor 2) holds for the Schrödinger problem as well.

In fact, we can replace the infimum over all A in the definition of $E(\beta, h, V)$ with a good a-priori bound on the field energy:

Corollary 1.2. *There exist universal constants $\varepsilon > 0$ and $\kappa_0 > 0$ such that if A_h is a sequence of vector potentials satisfying*

$$\lim_{h \rightarrow 0} h^{2-\varepsilon} \beta \int |\nabla \times A_h|^2 = 0, \quad (1.5)$$

then for any fixed smooth, compactly supported potential V , we have

$$\lim_{h \rightarrow 0, \beta h^2 \geq \kappa_0} h^{2-\varepsilon} \left| \text{Tr} (T_h(A_h) - V)_- + \beta \int |\nabla \times A_h|^2 - 2(2\pi h)^{-3} \iint [p^2 - V(q)]_- dp dq \right| = 0 \quad (1.6)$$

for the Pauli problem. The same result (without the prefactor 2) holds for the Schrödinger problem as well.

In [EFS1] we have also analyzed the semiclassical behavior of $E(\beta, h, V)$ in other regimes of the parameter β . The main motivation for a precise second order asymptotics in the specific regime $\beta h^2 \geq \text{const} > 0$ is that Theorem 1.1 is the main technical input for the proof of the Scott correction term of the ground state energy of large atoms and molecules in the limit when the nuclear charge Z tends to infinity. We refer to Section 2.3 of [EFS1] for the precise statement on the Scott correction with a self-generated magnetic field and for an explanation on its connection with semiclassical asymptotics. The actual proof of the Scott correction is given in a separate paper [EFS3].

2 Localized models

The semiclassical asymptotics is essentially a local issue. If the potential V has sufficient decay there will be no semiclassical contribution from infinity. It is an interesting question whether the decay needed for stability will ensure that there is no semiclassical contribution from infinity, but at this point we do not have a general proof of this. To separate the local semiclassics from the issue at infinity we introduce local versions of the energy.

Let ψ be a smooth function with $\text{supp } \psi \subset B(1)$, where in general $B(r)$ denotes the ball of radius r centered at the origin. We will always assume that $\|\psi\|_\infty \leq 1$ and ψ is identically 1 in a neighborhood of the origin. Denote by $\psi_r(x) = \psi(x/r)$. For any $r > 0$ define

$$E_r(\beta, h, V) := \inf_A \left[\text{Tr} [\psi_r(T_h(A) - V)\psi_r]_- + \beta \int_{\mathbb{R}^3} |\nabla \times A|^2 \right], \quad (2.1)$$

where we minimize over all $A \in H^1(\mathbb{R}^3; \mathbb{R}^3)$, or, equivalently, over all $A \in C_0^\infty(\mathbb{R}^3; \mathbb{R}^3)$. Alternatively, we may again restrict to vector potentials $A \in H^1(\mathbb{R}^3; \mathbb{R}^3)$ with $\nabla \cdot A = 0$ in (2.1) without changing the value of the infimum. Without loss of generality, we can always assume that V is supported in $B(r)$.

Here we have localized the particles but not the fields. We can also do both. Let us first note that if $\nabla \cdot A = 0$ then

$$\int_{\mathbb{R}^3} |\nabla \times A|^2 = \int_{\mathbb{R}^3} |\nabla \otimes A|^2, \quad (2.2)$$

where the integrand of the right contains all first derivatives, i.e. $|\nabla \otimes A|^2 = \sum_{ij=1}^3 |\partial_i A_j|^2$. This identity is easily seen using the Fourier transform. As the local version of the field energy we will use the localization of the integral on the right. For any $R \geq r > 0$ we thus set

$$E_{r,R}(\beta, h, V) := \inf_A \left[\text{Tr} [\psi_r(T_h(A) - V)\psi_r]_- + \beta \int_{B(R)} |\nabla \otimes A|^2 \right], \quad (2.3)$$

where we minimize over all $A \in H^1(B(R); \mathbb{R}^3)$, or, equivalently, over all $A \in C_0^\infty(\mathbb{R}^3; \mathbb{R}^3)$. The localized field energy is not fully gauge invariant, we therefore cannot restrict attention to divergence free vector potentials. We are however free to add a constant vector to A . Notice

that the integral of $|\nabla \otimes A|^2$ is taken on a larger ball $B(R)$ than $B(r)$ which contains the support of ψ_r . By virtue of gauge invariance and (2.2) we have

$$E_r = E_{r,\infty} := \lim_{R \rightarrow \infty} E_{r,R}.$$

By a simple rescaling we have

$$E_{r,R}(\beta, h, V) = r^{-2} E_{1,R/r}(r\beta, h, V_r),$$

where $V_r(x) = r^2 V(xr)$. It is thus enough to analyse the case $r = 1$.

The definition (2.1) is physically somewhat better motivated than (2.3) since it contains the energy of the magnetic field in the whole space and thus gives the correct magnetic interaction between the particles. The form (2.3) is however more useful if we want to localize all parts of the energy.

Another version of the localized energy would be

$$E'_{r,R}(\beta, h, V) := \inf_A \left[\text{Tr } \psi_r^2 [T_h(A) - V]_- + \beta \int_{B(R)} |\nabla \otimes A|^2 \right]. \quad (2.4)$$

This has the disadvantage of being more complicated to calculate as it requires knowledge of the operator $T_h(A) - V$ on the whole space, e.g. it is not enough to know V only on $B(r)$ or A only on $B(R)$. It has the advantage of not causing localization errors. Note that since ψ is assumed to be equal to 1 in a neighborhood of 0 we may identify

$$E(\beta, h, V) = \lim_{r \rightarrow \infty} E'_{r,\infty}(\beta, h, V) =: E'_{\infty,\infty}(\beta, h, V).$$

Finally we could also have defined the localized energy by introducing Dirichlet boundary conditions on the boundary of $B(r)$, i.e.,

$$E_{r,R}^D(\beta, h, V) := \inf_A \left[\text{Tr } [(T_h(A) - V)_{B(r),D}]_- + \beta \int_{B(R)} |\nabla \otimes A|^2 \right]. \quad (2.5)$$

We note that the leading order local semiclassical result (Theorem 1.3 in [ES]) was stated for Dirichlet boundary conditions.

In the main part of this work we will mainly use the global energy E in (1.2) or the localized energy $E_{r,R}$ in (2.3) but in the next section we will compare the local versions $E_r, E_{r,R}$, and $E'_{r,R}$. We will not discuss Dirichlet boundary conditions.

2.1 Comparison between the different localized energies

We first compare the energies $E_{r,R}$ and E_r .

Lemma 2.1. *There exists a universal constant C_0 such that for all $0 < r < R/2$ we have*

$$E_{r,R}(\beta, h, V) \leq E_r(\beta, h, V) \leq E_{r,R}((1 + C_0(r/R)^3)\beta, h, V). \quad (2.6)$$

This result holds for both the Pauli and Schrödinger operators.

Proof. The first inequality in (2.6) is trivial since $E_r = E_{r,\infty}$ and $E_{r,R}$ is clearly an increasing function of R .

To prove the second inequality we start from an approximate minimizing $A \in C_0^\infty$ for the energy $E_{r,R}$ on the right hand side of (2.6). By subtracting a constant vector from A we may assume that A has average 0 on the sphere $|x| = r$. We may, moreover, assume that A minimizes the Dirichlet integral $\int_{r < |x| < R} |\nabla \otimes A(x)|^2 dx$ given the boundary value of A on $|x| = r$. If not, we could improve the trial energy of A by replacing it on the set $r < |x| < R$ with the vector field that agrees with A for $|x| \leq r$ and minimizes $\int_{r < |x| < R} |\nabla \otimes A(x)|^2 dx$. As a trial vector field for the E_r we choose the field A' defined on all of \mathbb{R}^3 that agrees with A for $|x| \leq r$ and minimizes the integral $\int_{r < |x|} |\nabla \otimes A'(x)|^2 dx$. The vector fields A and A' in the region $|x| \geq r$ can be expressed in terms of the common boundary value of A on $|x| = r$. From the lemma below we see that there exists a universal constant C_0 such that

$$\int_{r < |x|} |\nabla \otimes A'(x)|^2 dx \leq (1 + C_0(r/R)^3) \int_{r < |x| < R} |\nabla \otimes A(x)|^2 dx.$$

Note that the constructed A' is not necessarily divergence free. Since A and A' agree on $|x| \leq r$ we obviously have

$$\int_{\mathbb{R}^3} |\nabla \times A'(x)|^2 dx \leq \int_{\mathbb{R}^3} |\nabla \otimes A'(x)|^2 dx \leq (1 + C_0(r/R)^3) \int_{|x| < R} |\nabla \otimes A(x)|^2 dx$$

and

$$\text{Tr} [\psi_r(T_h(A) - V)\psi_r]_- = \text{Tr} [\psi_r(T_h(A') - V)\psi_r]_-. \quad (2.7)$$

The second inequality of (2.6) follows from the last two observations. \square

We now give the simple estimate needed in the previous proof.

Lemma 2.2. *Assume $0 < 2r < R$ and let $S(r) = \{|x| = r\}$. Given $g \in L^2(S(r))$ with average 0. Let $f_1 \in H^1(B(R) \setminus B(r))$ and $f_2 \in H^1(\mathbb{R}^3 \setminus B(r))$ satisfy the boundary conditions $f_1|_{S(r)} = f_2|_{S(r)} = g|_{S(r)}$ and minimize the respective Dirichlet integrals*

$$\int_{B(R) \setminus B(r)} |\nabla f_1|^2, \quad \int_{\mathbb{R}^3 \setminus B(r)} |\nabla f_2|^2.$$

Then

$$\int_{\mathbb{R}^3 \setminus B(r)} |\nabla f_2|^2 \leq (1 + C_0(r/R)^3) \int_{B(R) \setminus B(r)} |\nabla f_1|^2,$$

for some universal constant C_0 .

Proof. By rescaling we may assume that $r = 1$. We know that f_1 is harmonic for $r < |x| < R$ and satisfies Neumann boundary conditions on the boundary $|x| = R$ and that f_2 is harmonic on $|x| > 1$ and tends to 0 at infinity. We can write

$$\int_{B(R) \setminus B(1)} |\nabla f_1|^2 = - \int_{S(1)} \bar{g} \partial_r f_1, \quad \int_{\mathbb{R}^3 \setminus B(1)} |\nabla f_2|^2 = - \int_{S(1)} \bar{g} \partial_r f_2.$$

We expand g in angular momentum eigenfunctions $g = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \alpha_{\ell m} Y_{\ell m}$. Since g has average 0, we have $\alpha_{00} = 0$. We also expand the harmonic functions

$$f_1(x) = \sum_{\ell m} (a_{1\ell m} |x|^\ell + b_{1\ell m} |x|^{-\ell-1}) Y_{\ell m}(x/|x|)$$

and

$$f_2(x) = \sum_{\ell m} b_{2\ell m} |x|^{-\ell-1} Y_{\ell m}(x/|x|).$$

The equality of the boundary conditions at $|x| = 1$ implies

$$b_{2\ell m} = a_{1\ell m} + b_{1\ell m} = \alpha_{\ell m}.$$

The Neumann condition at $|x| = R$ implies

$$\ell a_{1\ell m} = (\ell + 1) b_{1\ell m} R^{-2\ell-1}.$$

(Note all coefficients vanish for $\ell = 0$). Hence

$$b_{2\ell m} = (1 + \ell^{-1}(\ell + 1) R^{-2\ell-1}) b_{1\ell m}.$$

We thus obtain

$$- \int_{S(1)} \bar{g} \partial_r f_2 = 4\pi \sum_{\ell=1}^{\infty} \sum_{m=-\ell}^{\ell} (1 + \ell^{-1}(\ell + 1) R^{-2\ell-1})^2 |b_{1\ell m}|^2 (\ell + 1)$$

and

$$\begin{aligned} - \int_{S(1)} \bar{g} \partial_r f_1 &= 4\pi \sum_{\ell=1}^{\infty} \sum_{m=-\ell}^{\ell} (1 - R^{-2\ell-1})(1 + \ell^{-1}(\ell + 1) R^{-2\ell-1})(\ell + 1) |b_{1\ell m}|^2 \\ &\geq -(1 - 3R^{-3}) \int_{S(1)} \bar{g} \partial_r f_2. \end{aligned}$$

□

Now we compare $E_{r,R}$ and $E'_{r,R}$. Note that the only difference between $E_{r,R}$ and $E'_{r,R}$ is that in (2.4) ψ_r is outside the negative part. The following lemma shows that $E_{r,R}(\beta, h, V)$ and $E'_{r,R}(\beta, h, V)$ are essentially equivalent up to a term of high order in h (to appreciate the next result, recall that $E_{r,R}(\beta, h, V)$ is typically of order h^{-3}).

Lemma 2.3. *There exist universal constants $C_0, C_1, C_2 > 0$, such that*

$$\begin{aligned} E'_{r,R}(\beta, h, V) \leq E_{r,R}(\beta, h, V) \leq & E'_{r,R}((1 + C_0(r/R)^3 + \delta)\beta, h, V) \\ & + C_1 h^{-1}(\|V\|_{5/2}^{5/2} + r^{-2}) + C_2 h^2 \delta^{-3} \beta^{-3} (\|V\|_4^4 + r^{-5}) \end{aligned} \quad (2.8)$$

for all $\delta > 0$. The same result holds for the Schrödinger case, with $\delta = C_0 = C_2 = 0$, i.e.

$$E'_{r,R}(\beta, h, V) \leq E_{r,R}(\beta, h, V) \leq E'_{r,R}(\beta, h, V) + C_1 h^{-1}(\|V\|_{5/2}^{5/2} + r^{-2}). \quad (2.9)$$

Note that norms of V in this Lemma are in the whole space.

Proof. Let $H = H_h(A) = T_h(A) - V$. Since

$$\text{Tr} [\psi_r H \psi_r]_- \geq \text{Tr} [\psi_r [H]_- \psi_r]_- = \text{Tr} \psi_r [H]_- \psi_r,$$

the first bound in (2.8) is trivial.

In order to prove the second inequality, we write $\gamma := \mathbf{1}_{(-\infty, 0]}(H)$ and calculate,

$$\begin{aligned} \text{Tr} \psi_r^2 [H]_- &= \frac{1}{2} \text{Tr} (\psi_r^2 [H]_- + [H]_- \psi_r^2) = \frac{1}{2} \text{Tr} ((\psi_r^2 H + H \psi_r^2) \gamma) \\ &= \frac{1}{2} \text{Tr} ([H, \psi_r], \psi_r + 2\psi_r H \psi_r) \gamma. \end{aligned} \quad (2.10)$$

Therefore, by the variational principle, and since $[[H, \psi_r], \psi_r] = -2h^2(\nabla \psi_r)^2$

$$\text{Tr} [\psi_r H \psi_r]_- \leq \text{Tr} \psi_r^2 [H]_- + h^2 \text{Tr} (\nabla \psi_r)^2 \gamma. \quad (2.11)$$

In order to estimate the last term we apply a Lieb-Thirring inequality from [LLS]:

Theorem 2.4. [LLS] *There exist a universal constant C such that for the semiclassical Pauli operator $T_h(A) - V$ with a potential $V \in L^{5/2}(\mathbb{R}^3) \cap L^4(\mathbb{R}^3)$ and magnetic field $B = \nabla \times A \in L^2(\mathbb{R}^3)$ we have*

$$\text{Tr} [T_h(A) - V]_- \geq -Ch^{-3} \int [V]_+^{5/2} - C \left(h^{-2} \int |B|^2 \right)^{3/4} \left(\int [V]_+^4 \right)^{1/4}. \quad (2.12)$$

Using $\text{Tr} H \gamma \leq 0$ and applying (2.12) to the operator $H - (\nabla \psi_r)^2$, we obtain

$$\begin{aligned} -\text{Tr} (\nabla \psi_r)^2 \gamma &\geq \text{Tr} (H - (\nabla \psi_r)^2) \gamma \\ &\geq -Ch^{-3} \int [V + (\nabla \psi_r)^2]_+^{5/2} - C \left(h^{-2} \int_{\mathbb{R}^3} |\nabla \times A|^2 \right)^{3/4} \left(\int [V + (\nabla \psi_r)^2]_+^4 \right)^{1/4} \\ &\geq -Ch^{-3} \left(\int [V]_+^{5/2} + r^{-2} \right) - C \delta^{-3} \beta^{-3} \left(\int [V]_+^4 + r^{-5} \right) - \delta \beta h^{-2} \int_{\mathbb{R}^3} |\nabla \times A|^2. \end{aligned} \quad (2.13)$$

From (2.11) we thus have

$$\begin{aligned} E_{r,R}(\beta, h, V) &\leq \inf_A \left[\text{Tr } \psi_r^2 [T_h(A) - V]_- + (1 + \delta)\beta \int_{\mathbb{R}^3} |\nabla \times A|^2 \right] \\ &\quad + Ch^{-1} \left(\int [V]_+^{5/2} + r^{-2} \right) + Ch^2 \delta^{-3} \beta^{-3} \left(\int [V]_+^4 + r^{-5} \right). \end{aligned}$$

Exactly as in the upper bound in Lemma 2.1, we can replace $\int_{\mathbb{R}^3} |\nabla \times A|^2$ with $\int_{B(R)} |\nabla \otimes A|^2$ at the expense of increasing β by a factor. This proves Lemma 2.3 for the Pauli case. For the Schrödinger case we can use the non-magnetic Lieb-Thirring inequality, i.e. the second line of (2.13) simplifies to

$$-\text{Tr } (\nabla \psi_r)^2 \gamma \geq -Ch^{-3} \int [V + (\nabla \psi_r)^2]_+^{5/2}$$

and the rest of the argument is the same. \square

3 Refined local semiclassics with scales

We consider a local version of Theorem 1.4 for a model problem living in the ball $B(\ell)$ of radius $\ell > 0$. Note that not only the Hamiltonian but also the magnetic field has been localized, albeit on a twice bigger ball. We introduce two scaling parameters, ℓ and f , that describe the lengthscale and the strength of the potential and we follow the dependence of the error term on these parameters. This scale invariant formulation will be convenient for the multiscale analysis in [EFS3] and also in the reduction of the following theorem to its special case, Theorem 4.1. Readers who are interested only in the semiclassical aspect of the result can think of $f = \ell = 1$.

Theorem 3.1 (Semiclassical asymptotics). *There exist universal constants $n_0 \in \mathbf{N}$ and $\varepsilon > 0$ such that the following is satisfied. Let $\kappa_0, f, \ell, h_0 > 0$ and let $\kappa \leq \kappa_0 f^{-2} \ell^{-1}$. Let $\psi \in C_0^\infty(\mathbb{R}^3)$ with $\text{supp } \psi \subset B(\ell)$ and let $V \in C^\infty(\overline{B}(\ell))$ be a real valued potential satisfying*

$$|\partial^n \psi| \leq C_n \ell^{-|n|}, \quad |\partial^n V| \leq C_n f^2 \ell^{-|n|} \quad (3.1)$$

for every multiindex n with $|n| \leq n_0$. Then for the Pauli operator $H_h(A) := T_h(A) - V$,

$$\begin{aligned} \left| \inf_A \left(\text{Tr } [\psi H_h(A) \psi]_- + \frac{1}{\kappa h^2} \int_{B(2\ell)} |\nabla \otimes A|^2 \right) - 2(2\pi h)^{-3} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \psi(q)^2 [p^2 - V(q)]_- dq dp \right| \\ \leq Ch^{-2+\varepsilon} f^{4-\varepsilon} \ell^{2-\varepsilon} \quad (3.2) \end{aligned}$$

for any $h \leq h_0 f \ell$. The constant C depends only on κ_0, h_0 and on the constants C_n , in (3.1). The factor 2 in front of the semiclassical term accounts for the spin and it is present only for the Pauli case.

Remark 1. For convenience, we introduced a new parameter $\kappa = \beta^{-1}h^{-2}$ instead of β . In the limit we consider, $h \rightarrow \infty$, $\beta h^2 \geq \text{const} > 0$, the new parameter κ will remain bounded uniformly. We note that the constant factor β in front of the magnetic energy does not necessarily have to scale as h^{-2} (see [EFS1] for other scalings) but our choice here is dictated by the application to the Scott correction. Similar results may be proven with a more general coefficient $\beta \sim h^{-\gamma}$ with a certain range of γ and the exponent of the error term will be $\varepsilon = \varepsilon(\gamma)$. We will not pursue the most general result in this paper.

Remark 2. By variation of κ , we obtain from Theorem 3.1 the following estimate

$$\frac{1}{\kappa h^2} \int_{B(2\ell)} |\nabla \otimes A|^2 \leq Ch^{-2+\varepsilon} f^{4-\varepsilon} \ell^{2-\varepsilon}, \quad (3.3)$$

for (near) minimizing vector potentials A .

The following result can be viewed as a partial converse to (3.3) as it estimates the semiclassical error in terms of the magnetic field. Note that the assumption in (3.4) below is much weaker than (3.3).

Theorem 3.2. *Let the assumptions be as in Theorem 3.1 and assume that A satisfies the bound*

$$\int_{B(2\ell)} |\nabla \otimes A|^2 \leq Ch^{-2} f^4 \ell^3. \quad (3.4)$$

Then, with ε from Theorem 3.1 we have

$$\begin{aligned} Ch^{-2} f^3 \ell^{3/2} \left\{ \int_{B(2\ell)} |\nabla \otimes A|^2 \right\}^{1/2} + Ch^{-1} f^3 \ell \\ \geq \text{Tr} [\psi H_h(A) \psi]_- - 2(2\pi h)^{-3} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \psi(q)^2 [p^2 - V(q)]_- dq dp \\ \geq Ch^{-2+\varepsilon} f^{4-\varepsilon} \ell^{2-\varepsilon} - Ch^{-2} f^2 \ell \int_{B(2\ell)} |\nabla \otimes A|^2, \end{aligned} \quad (3.5)$$

where the constants may depend on h_0 and κ_0 and on the constant in (3.4).

3.1 Proof of the Main Theorem 1.1

Using the local semiclassical asymptotics Theorem 3.1 it is an easy localization argument to prove the global result for compactly supported potentials.

Recall the choice of a smooth cutoff function ψ from Section 2. Let $f = 1$ and $\ell \geq 1$ sufficiently large so that $\psi_\ell(x) := \psi(x/\ell) \equiv 1$ on the support of V .

The upper bound in Theorem 1.1 is obtained by setting $A = 0$ and using the first inequality in Lemma 2.3 (with $R = \infty$)

$$E(\beta, h, V) \leq 2\text{Tr} [-h^2\Delta - V]_- \leq 2\text{Tr} \psi_\ell [-h^2\Delta - V]_- \psi_\ell \leq 2\text{Tr} [\psi_\ell (-h^2\Delta - V) \psi_\ell]_-,$$

where the traces are on $L^2(\mathbb{R}^3)$ and the factor 2 accounts for the spin. The upper bound now follows from the main result of [SS] which is formulated for $\ell = 1$, but it clearly extends to any value of ℓ :

Theorem 3.3 ([SS, Theorem 12]). *Let $d \geq 3$ and $\psi \in C_0^{d+4}(\mathbb{R}^d)$ be supported in a ball B of radius 1 and $V \in C^3(\overline{B})$ be a real function. Let $H = -h^2\Delta - V$, $h > 0$, acting on $L^2(\mathbb{R}^d)$. Then,*

$$\left| \text{Tr}_{L^2(\mathbb{R}^d)} [\psi H \psi]_- - (2\pi h)^{-d} \int_{\mathbb{R}^d \times \mathbb{R}^d} \psi^2(q) [p^2 - V(q)]_- dp dq \right| \leq Ch^{-d+6/5}. \quad (3.6)$$

The constant $C > 0$ here depends only on d , $\|\psi\|_{C^{d+4}}$ and $\|V\|_{C^3}$.

For the lower bound in Theorem 1.1 we use the IMS localization with a partition of unity $\psi_\ell^2 + \tilde{\psi}_\ell^2 \equiv 1$ and we borrow a small fraction of the kinetic energy to control the localization error. We have

$$T_h(A) - V \geq (1 - \delta)\psi_\ell(T_h(A) - V_\delta)\psi_\ell + \delta[T_h(A) - \delta^{-1}h^2I_\ell] \quad (3.7)$$

with $\delta \in (0, \frac{1}{4})$, $I_\ell := (\nabla\psi_\ell)^2 + (\nabla\tilde{\psi}_\ell)^2$ and $V_\delta = (1 - \delta)^{-1}V$. Here we dropped the term $\tilde{\psi}_\ell(T_h(A) - V_\delta)\tilde{\psi}_\ell$ that is positive since $V_\delta = 0$ on the support of $\tilde{\psi}_\ell$. The second term in (3.7) is estimated by the magnetic Lieb-Thirring inequality similarly to (2.13):

$$\text{Tr} [T_h(A) - \delta^{-1}h^2I_\ell]_- \geq -Ch^2\delta^{-5/2} - C\beta^{-3}h^2\delta^{-4} - \beta \int |\nabla \times A|^2,$$

where the constants depend on V and ℓ . Using $\beta h^2 \geq \kappa_0$ and assuming $h \leq 1$, we can combine the two error terms to obtain

$$E(\beta, h, V) \geq (1 - \delta)E'_{\ell, \infty}(\beta, h, V_\delta) - Ch^2\delta^{-3} \geq E_{\ell, 2\ell}(\beta/2, h, V_\delta) - Ch^2\delta^{-3} - Ch^{-1}.$$

In the last step we used the second inequality from (2.8) with $R = \infty$ and then the monotonicity of $E_{\ell, R} < 0$ in R . The energy $E_{\ell, 2\ell}(\beta/2, h, V_\delta)$ is estimated in (3.2) (with $\kappa = 2\beta^{-1}h^{-2}$) and we get

$$E(\beta, h, V) \geq 2(2\pi h)^{-3} \int_{\mathbb{R}^3 \times \mathbb{R}^3} [p^2 - V_\delta(q)]_- dp dq - Ch^{-2+\varepsilon} - Ch^2\delta^{-3},$$

where we used again that $\psi_\ell \equiv 1$ on the support of V_δ . It is easy to see that

$$\int_{\mathbb{R}^3 \times \mathbb{R}^3} [p^2 - V_\delta(q)]_- dp dq = \int_{\mathbb{R}^3 \times \mathbb{R}^3} [p^2 - V(q)]_- dp dq + O(\delta)$$

and finally, choosing $\delta = h^{1+\varepsilon}$ we obtain an error term $Ch^{-2+\varepsilon}$ assuming $\varepsilon \leq 1/4$. This completes the proof of Theorem 1.1. \square

4 Refined local semiclassics with lower bound

The main technical result of this paper is the following version of Theorem 3.1 where additionally a lower bound on V , namely (4.2) is assumed. Furthermore, we impose the condition that $\nabla \cdot A = 0$.

Theorem 4.1 (Semiclassical asymptotics). *There exist universal constants $n_0 \in \mathbf{N}$ and $\varepsilon > 0$ such that the following is satisfied. Let $\kappa_0, f, \ell, h_0 > 0$ and let $\kappa \leq \kappa_0 f^{-2} \ell^{-1}$. Let $\psi \in C_0^\infty(\mathbb{R}^3)$ with $\text{supp } \psi \subset B(\ell)$ and let $V \in C^\infty(\overline{B}(\ell))$ be a real valued potential satisfying*

$$|\partial^n \psi| \leq C_n \ell^{-|n|}, \quad |\partial^n V| \leq C_n f^2 \ell^{-|n|} \quad (4.1)$$

for every multiindex n with $|n| \leq n_0$, and for some $c_0 > 0$ let

$$\inf\{V(x) : x \in \overline{B}(\ell)\} \geq c_0 f^2. \quad (4.2)$$

Then

$$\left| \inf'_A \left(\text{Tr} [\psi H_h(A) \psi]_- + \frac{1}{\kappa h^2} \int_{B(2\ell)} |\nabla \otimes A|^2 \right) - 2(2\pi h)^{-3} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \psi(q)^2 [p^2 - V(q)]_- dq dp \right| \leq C h^{-2+\varepsilon} f^{4-\varepsilon} \ell^{2-\varepsilon} \quad (4.3)$$

for any $h \leq h_0 f \ell$. Here \inf'_A denotes that the infimum is taken over all $A \in H^1(\mathbb{R}^3)$ satisfying that

$$\nabla \cdot A = 0, \quad \text{on } B(5\ell/4). \quad (4.4)$$

The constant C depends only on κ_0 , h_0 and on the constants C_n , and c_0 in (4.1) and (4.2). The factor 2 in front of the semiclassical term accounts for the spin and it is present only for the Pauli case.

Note that this theorem is formulated in a scale invariant way, so it will be sufficient to prove it for $f = \ell = 1$.

We first show that the condition $\nabla \cdot A = 0$ is irrelevant for the statement of Theorem 4.1, i.e. one gets the same result by dropping the condition $\nabla \cdot A = 0$.

Theorem 4.2. *Suppose that Theorem 4.1 holds, where the infimum is taken over all A with $\nabla \cdot A = 0$ on $B(5\ell/4)$. Then Theorem 4.1 also holds where the infimum is taken over all A .*

Proof. Clearly the unrestricted infimum is smaller than the one with the condition $\nabla \cdot A = 0$ imposed. We will prove the opposite inequality, namely that there exists $C > 0$ such that

$$\inf'_A \left(\text{Tr} [\psi H_h(A) \psi]_- + \frac{1}{C \kappa h^2} \int_{B(2\ell)} |\nabla \otimes A|^2 \right) \leq \inf_A \left(\text{Tr} [\psi H_h(A) \psi]_- + \frac{1}{\kappa h^2} \int_{B(2\ell)} |\nabla \otimes A|^2 \right), \quad (4.5)$$

where \inf'_A means that we take the restricted infimum over A with $\nabla \cdot A = 0$ on $B(5\ell/4)$. Since the constant κ is arbitrary this implies the result.

For an arbitrary $A \in H^1$, we can add a constant to A in order to get, by a Poincaré inequality, that

$$\ell^{-2} \int_{B(2\ell)} A^2 \leq C \int_{B(2\ell)} |\nabla \otimes A|^2. \quad (4.6)$$

Clearly, this additive constant does not change the energy, i.e. on the right hand side of (4.5) we can assume that A satisfies (4.6).

Choose a localization function $\chi \in C_0^\infty(B(3\ell/2))$, $\chi = 1$ on $B(5\ell/4)$. Define A_χ to satisfy

$$\nabla \times A_\chi = B_\chi := \nabla \times (\chi A), \quad \nabla \cdot A_\chi = 0. \quad (4.7)$$

This system defines A_χ up to an additive constant that we will choose in order to be able to apply the Poincaré inequality below. Finally, define a vector field A' by $A' := \chi A_\chi$, then clearly $\nabla \cdot A' = 0$ on $B(5\ell/4)$.

Then,

$$\text{Tr} [\psi H_h(A) \psi]_- = \text{Tr} [\psi H_h(\chi A) \psi]_- = \text{Tr} [\psi H_h(A_\chi) \psi]_- = \text{Tr} [\psi H_h(A') \psi]_-, \quad (4.8)$$

where the middle equality follows from the gauge equivalence of A_χ and χA , and the other two follow from the fact that $\chi \equiv 1$ on $\text{supp } \psi$. Also, using the Poincaré inequality twice, once for A (4.6) and once for A_χ , we have

$$\begin{aligned} \int_{B(2\ell)} |\nabla \otimes A'|^2 &\leq \int_{B(2\ell)} |\nabla \otimes A_\chi|^2 + C\ell^{-2} \int_{B(2\ell)} |A_\chi|^2 \leq C \int_{B(2\ell)} |\nabla \otimes A_\chi|^2 \\ &\leq C \int_{\mathbb{R}^3} |\nabla \otimes A_\chi|^2 = C \int_{\mathbb{R}^3} B_\chi^2 \leq C \left(\ell^{-2} \int_{B(2\ell)} A^2 + \int_{B(2\ell)} |\nabla \times A|^2 \right) \\ &\leq C \int_{B(2\ell)} |\nabla \otimes A|^2. \end{aligned} \quad (4.9)$$

□

4.1 Multiscaling

To prove that Theorem 3.1 follows from Theorem 4.2 requires to perform a multiscale decomposition around the sets where V is too small and it violates (4.2). We present the setup for multiscaling for general potentials that will also be applicable for resolution of Coulomb like singularities.

We will assume that the potential has a multiscale structure. Intuitively, this means that there exist two scaling functions, $f, \ell : \mathbb{R}^3 \rightarrow \mathbb{R}_+$ such that for any $u \in \mathbb{R}^3$, within the ball

$B_u(\ell(u))$ centered at u with radius $\ell(u)$, the size of V is of order $f^2(u)$ and V varies on scale $\ell(u)$. Moreover, we also require that the continuous family of balls $B_u(\ell(u))$ supports a regular partition of unity. The following lemma states this condition precisely. This statement was proved in Theorem 22 of [SS] with an explicit construction¹.

We will use the notation $B_x(r)$ for the ball of radius r and center at x and if $x = 0$, we use $B(r) = B_0(r)$.

Lemma 4.3. *Fix a cutoff function $\psi \in C_0^\infty(\mathbb{R}^3)$ supported in the unit ball $B(1)$ satisfying $\int \psi^2 = 1$. Let $\ell : \mathbb{R}^3 \rightarrow (0, 1]$ be a C^1 function with $\|\nabla \ell\|_\infty < 1$. Let $J(x, u)$ be the Jacobian of the map $u \mapsto (x - u)/\ell(u)$ and we define*

$$\psi_u(x) = \psi\left(\frac{x - u}{\ell(u)}\right) \sqrt{J(x, u)} \ell(u)^{3/2}.$$

Then, for all $x \in \mathbb{R}^3$,

$$\int_{\mathbb{R}^3} \psi_u(x)^2 \ell(u)^{-3} du = 1, \quad (4.10)$$

and for all multi-indices $n \in \mathbf{N}^3$ we have

$$\|\partial^n \psi_u\|_\infty \leq C_n \ell(u)^{-|n|}, \quad |n| = n_1 + n_2 + n_3, \quad (4.11)$$

where C_n depends on the derivatives of ψ but is independent of u .

We will require that the potential satisfies

$$|\partial^n V(u)| \leq C_n f(u)^2 \ell(u)^{-|n|} \quad (4.12)$$

for all $n \in \mathbf{N}^3$ uniformly in u in some domain $\Omega \subset \mathbb{R}^3$. In applications, Ω will exclude an h -neighborhood of the core of the Coulomb potentials.

For brevity, we will often use $\ell_u = \ell(u)$ and $f_u = f(u)$.

4.2 Proof of Theorem 3.1

We now show how Theorem 3.1 follows from Theorem 4.1.

Proof of Theorem 3.1. By Theorem 4.2 we may forget about the condition (4.4) in Theorem 4.1 and consider the infimum over all $A \in H^1$. Moreover, since (3.2) is local, we may assume without loss of generality that V has compact support contained in $B(5\ell/4)$. After these remarks, Theorem 3.1 would follow from Theorem 4.1 once we have shown that the additional condition (4.2) in Theorem 4.1 can be removed.

Since the statement of Theorem 3.1 is scale invariant we may also assume that $f = \ell = 1$ in the statement of that theorem. We will apply Theorem 4.1 and the partition of unity Lemma 4.3 with a different choice of f and ℓ .

¹Multiscaling was introduced in semiclassical problems in [IS] (see also [Sob])

The statement of Theorem 4.1 consists of a lower and an upper bound on the total quantum energy. Since the proof of the upper bound (see (5.1)) does not use the condition (4.2), the upper bound in Theorem 3.1 follows immediately, so we only need to prove the lower bound. Define the smooth functions

$$\ell(x) = f(x)^2 := \frac{1}{K} (V(x)^2 + h^{2\alpha})^{1/2} \quad (4.13)$$

with some positive exponent with $2/5 < \alpha < 1/2$ and recall the notation $\ell_x = \ell(x)$ and $f_x = f(x)$. Here $K > 0$ (independent of h , but depending on V and h_0 given in Theorem 3.1) is chosen so large that

$$\|\nabla \ell\|_\infty < 1/4, \quad \ell_u \leq 1/4, \quad u \in B(2). \quad (4.14)$$

By Lemma 4.3 there is a partition of unity ψ_u associated to ℓ . Inserting this partition of unity, we have for sufficiently small values of h that

$$\begin{aligned} \text{Tr} [\psi(T_h(A) - V)\psi]_- &+ \frac{1}{\kappa h^2} \int_{B(2)} |\nabla \otimes A|^2 dx \\ &= \text{Tr} \left[\int_{B(3/2)} \frac{du}{\ell_u^3} \psi \left(\psi_u [T_h(A) - V] \psi_u - h^2 |\nabla \psi_u|^2 \right) \psi \right]_- + \frac{1}{\kappa h^2} \int_{B(2)} |\nabla \otimes A|^2 \\ &\geq \text{Tr} \left[\int_{B(3/2)} \frac{du}{\ell_u^3} \tilde{\psi}_u [T_h(A) - V - Ch^2 \ell_u^{-2}] \tilde{\psi}_u \right]_- + \frac{1}{\kappa h^2} \int_{B(2)} |\nabla \otimes A|^2 \\ &\geq \int_{u \in B(3/2)} \left\{ \text{Tr} [\tilde{\psi}_u (T_h(A) - V - Ch^2 \ell_u^{-2}) \tilde{\psi}_u]_- + \frac{1}{\kappa' h^2} \int_{B_u(2\ell_u)} |\nabla \otimes A|^2 dx \right\} \frac{du}{\ell_u^3} \end{aligned} \quad (4.15)$$

with $\tilde{\psi}_u := \psi_u \psi$ and κ' a fixed constant times κ . We also used $\text{Tr} [\int O_u du]_- \geq \int \text{Tr} [O_u]_- du$ for any continuous family of operators O_u . In arriving at (4.15) we reallocated the localization error by using

$$\frac{\ell_u}{2} \leq \ell_x \leq \frac{3\ell_u}{2}, \quad \text{for all } x \in B_u(2\ell_u) \quad (4.16)$$

which follows from $\|\nabla \ell\|_\infty \leq 1/4$. We also reallocated the magnetic energy by using the estimate

$$\begin{aligned} \int_{u \in B(3/2)} \int_{B_u(2\ell_u)} |\nabla \otimes A(x)|^2 dx \frac{du}{\ell_u^3} &\leq \int_{x \in B(2)} \int_{u \in B_x(4\ell_x)} |\nabla \otimes A(x)|^2 (2\ell_x/3)^{-3} du dx \\ &= C \int_{x \in B(2)} |\nabla \otimes A(x)|^2 dx, \end{aligned} \quad (4.17)$$

where we again used (4.16).

Consider now $u \in B(3/2)$ and suppose first that $|V(u)| \geq h^\alpha$. Then, if K in the definition of f, ℓ (4.13) is chosen sufficiently large, we have by the uniform bounds on the derivatives

of V that $|V(x)| \geq |V(u)|/2 \geq f_u^2/4$ for all $x \in B_u(\ell_u)$. So (4.2) is satisfied (with $c_0 = 1/4$). Using (4.11), the estimates in (4.1) are also easily seen to be satisfied for the cutoff function $\tilde{\psi}_u$ and for the potential $V + Ch^2\ell_u^{-2}$ with $\ell = \ell_u$ and $f = f_u$ (here we use that $\alpha < 2/3$ and that K may depend on h_0). We can therefore conclude by Theorem 4.2 that for any A ,

$$\begin{aligned} & \int_{\{u \in B(3/2): |V(u)| \geq h^\alpha\}} \left\{ \text{Tr} [\tilde{\psi}_u(T_h(A) - V - Ch^2\ell_u^{-2})\tilde{\psi}_u]_- + \frac{1}{\kappa'h^2} \int_{B_u(2\ell_u)} |\nabla \otimes A|^2 dx \right\} \frac{du}{\ell_u^3} \\ & \geq \int_{\{u \in B(3/2): |V(u)| \geq h^\alpha\}} \left\{ \frac{2}{(2\pi h)^3} \iint \tilde{\psi}_u(q)^2 [p^2 - V(q) - Ch^2\ell_u^{-2}]_- dq dp - Ch^{-2+\varepsilon} \ell_u^{4-3\varepsilon/2} \right\} \frac{du}{\ell_u^3} \\ & \geq 2(2\pi h)^{-3} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \psi(q)^2 [p^2 - V(q)]_- dq dp - Ch^{2-2\alpha} h^{-3} - Ch^{-2+\varepsilon} \int_{B(3/2)} \ell_u^{1-3\varepsilon/2} du, \quad (4.18) \end{aligned}$$

where we used (4.10) and that $h^2\ell_u^{-2} \leq Ch^{2-2\alpha}$ to get the last inequality. Since ℓ is bounded and $\alpha < 1/2$, both error terms in (4.18) are acceptable.

For the set of u 's where $V(u)$ is small, i.e., $|V(u)| \leq h^\alpha$, we use the magnetic Lieb-Thirring inequality. We introduce $A' = \chi(A - c)$, where $\chi \in C_0^\infty(B_u(2\ell_u))$, $\chi = 1$ on $B_u(\ell_u)$ and $|\nabla \chi| \leq C/\ell_u$. Here $c = \int_{B_u(2\ell_u)} A$. Then we have, using the Poincaré inequality,

$$\int |\nabla \otimes A'|^2 \leq C \int_{B_u(2\ell_u)} \left(\ell_u^{-2}(A - c)^2 + |\nabla \otimes A|^2 \right) \leq C' \int_{B_u(2\ell_u)} |\nabla \otimes A|^2.$$

So we get

$$\begin{aligned} & \text{Tr} [\tilde{\psi}_u(T_h(A) - V - Ch^2\ell_u^{-2})\tilde{\psi}_u]_- + \frac{1}{\kappa'h^2} \int_{B_u(2\ell_u)} |\nabla \otimes A|^2 \\ & \geq \text{Tr} [T_h(A') - (V + Ch^2\ell_u^{-2})\mathbf{1}_{B_u(\ell_u)}]_- + \frac{1}{\kappa'h^2} \int_{B_u(2\ell_u)} |\nabla \otimes A|^2 \\ & \geq -C \left\{ h^{-3} \int_{B_u(\ell_u)} [V + Ch^2\ell_u^{-2}]_+^{5/2} + \left(\int_{B_u(\ell_u)} [V + Ch^2\ell_u^{-2}]_+^4 \right)^{1/4} \left(h^{-2} \int_{B_u(2\ell_u)} |\nabla \otimes A|^2 \right)^{3/4} \right\} \\ & \quad + \frac{1}{\kappa'h^2} \int_{B_u(2\ell_u)} |\nabla \otimes A|^2 \\ & \geq -C(\kappa') \left\{ h^{-3} \int_{B_u(\ell_u)} [V + Ch^2\ell_u^{-2}]_+^{5/2} + \int_{B_u(\ell_u)} [V + Ch^2\ell_u^{-2}]_+^4 \right\} \\ & \geq -C(\kappa') h^{-3+5\alpha/2} \ell_u^3, \quad (4.19) \end{aligned}$$

since $|V(u)| \leq h^\alpha$ and $\ell_u \sim h^\alpha$, so we get $|V(x)| \leq |V(u)| + C\ell_u \leq Ch^\alpha$ for any $x \in B_u(\ell_u)$. In summary, we have

$$\begin{aligned} & \int_{\{u \in B(3/2): |V(u)| \leq h^\alpha\}} \left\{ \text{Tr} [\tilde{\psi}_u(T_h(A) - V - Ch^2\ell_u^{-2})\tilde{\psi}_u]_- + \frac{1}{\kappa'h^2} \int_{B_u(2\ell_u)} |\nabla \otimes A|^2 \right\} \frac{du}{\ell_u^3} \\ & \geq -Ch^{-3+5\alpha/2}. \quad (4.20) \end{aligned}$$

Since $\alpha > 2/5$, this error term is acceptable, in fact $\alpha = 4/9$ optimizes the errors from (4.18) and (4.20), which shows that $\varepsilon < 1/9$. Thus the final ε in Theorem 3.1 is the minimum of $1/9$ and the ε obtained in Theorem 4.1. This finishes the proof of the lower bound and therefore the proof of Theorem 3.1. \square

4.3 Proof of Theorem 3.2

We now show how Theorem 3.2 follows from Theorem 3.1.

Proof of Theorem 3.2. By the argument given in the proof of Theorem 4.2, we may assume that $\nabla \cdot A = 0$ on a neighborhood of $\text{supp } \psi$. Also, by a rescaling we may assume that $f = \ell = 1$.

The lower bound in (3.5) follows directly from Theorem 3.1. The upper bound in (3.5) will be constructed using an explicit trial state. Define

$$\gamma := \int \chi_u \exp(-ic_u x) \gamma_u \exp(-ic_u x) \chi_u \frac{du}{L_0^3} \quad (4.21)$$

with a length scale $L_0 \leq 1$ that will be optimized at the end of the proof. Here $\chi_u(x) = \chi((x - u)/L_0)$, with $\chi \in C_0^\infty(B(1))$ a real, positive function with $\int \chi^2 = 1$. Clearly χ_u is supported in the ball $B_u(L_0)$. We choose the parameter $c_u := \int_{B_u(L_0)} A$. Also

$$\gamma_u = \mathbf{1}_{(-\infty, 0]}(\chi_u \psi H_h(A = 0) \psi \chi_u).$$

Notice that γ_u is real and acts like a scalar in spinor space. Therefore the contribution of the cross terms $[\boldsymbol{\sigma} \cdot (-ih\nabla)][\boldsymbol{\sigma} \cdot A] + [\boldsymbol{\sigma} \cdot A][\boldsymbol{\sigma} \cdot (-ih\nabla)]$ on $\psi \chi_u \gamma_u \chi_u \psi$ vanishes and we get

$$\begin{aligned} \text{Tr } \psi H_h(A) \psi \gamma &= \int \text{Tr } [\chi_u \psi H_h(A - c_u) \psi \chi_u \gamma_u] \frac{du}{L_0^3} \\ &= \int_{B(2)} \left(\text{Tr } [\chi_u \psi H_h(A = 0) \psi \chi_u]_- + \text{Tr } [\chi_u^2 \psi^2 (A - c_u)^2 \gamma_u] \right) \frac{du}{L_0^3}. \end{aligned}$$

The du integration can be restricted to $B(2)$ by the support properties of ψ and χ_u and by $L_0 \leq 1$. By a rescaling to a ball of unit size and an application of an optimal semiclassical result (recalled below as Theorem 5.6) we get that

$$\text{Tr } [\chi_u \psi H_h(A = 0) \psi \chi_u]_- \leq 2(2\pi h)^{-3} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \chi_u^2(q) \psi(q)^2 [p^2 - V(q)]_- dq dp + C(h/L_0)^{-1}, \quad (4.22)$$

with a constant C independent of u . Performing the integration over u we will therefore get the desired upper bound if we can estimate the A^2 term as well. For this, we apply Hölder,

Lieb-Thirring and Sobolev inequalities to get (with $\tilde{\gamma}_u := \chi_u \psi \gamma_u \psi \chi_u$ and $\tilde{\rho}_u$ the associated density that is supported on $B_u(L_0)$),

$$\begin{aligned}
\int (A - c_u)^2 \tilde{\rho}_u &\leq \left(\int_{B_u(L_0)} (A - c_u)^5 \right)^{2/5} \left(\int \tilde{\rho}_u^{5/3} \right)^{3/5} \\
&\leq \left(\int_{B_u(L_0)} (A - c_u)^6 \right)^{3/10} \left(\int_{B_u(L_0)} (A - c_u)^2 \right)^{1/10} \left(\int \tilde{\rho}_u^{5/3} \right)^{3/5} \\
&\leq \left(\int_{B_u(L_0)} |\nabla \otimes A|^2 \right)^{9/10} \left(L_0^2 \int_{B_u(L_0)} |\nabla \otimes A|^2 \right)^{1/10} \left(\int \tilde{\rho}_u^{5/3} \right)^{3/5} \\
&\leq CL_0^{1/5} \|\nabla \otimes A\|_{L^2(B_u(L_0))}^2 \left(h^{-2} \text{Tr} [D^2 \tilde{\gamma}_u] \right)^{3/5},
\end{aligned}$$

where we defined $D := -ih\nabla$ for brevity. Here we used the choice of c_u and the Poincaré inequality in $B_u(L_0)$ to control $A - c_u$ in L^2 by $L_0 \|\nabla \otimes A\|_{L^2(B_u(L_0))}$.

Since we have the following bound, which we will prove below,

$$\text{Tr} [D^2 \tilde{\gamma}_u] \leq Ch^{-3} L_0^3, \quad (4.23)$$

we can estimate

$$\begin{aligned}
\int_{B(2)} \text{Tr} [\chi_u^2 \psi^2 (A - c_u)^2 \gamma_u] \frac{du}{L_0^3} &\leq CL_0^2 h^{-3} \int \|\nabla \otimes A\|_{L^2(B_u(L_0))}^2 \frac{du}{L_0^3} \\
&\leq CL_0^2 h^{-3} \int_{B(2)} |\nabla \otimes A|^2.
\end{aligned} \quad (4.24)$$

Now we choose L_0 by optimizing the error terms $CL_0^{-3}(h/L_0)^{-1}$ from (4.22) and from (4.24). Taking into account $L_0 \leq 1$, the result is the choice

$$L_0 = \min \left\{ 1, h^{1/2} \left(\int_{B(2)} |\nabla \otimes A|^2 \right)^{-1/4} \right\}. \quad (4.25)$$

Therefore, we obtain the desired upper bound in (3.5).

It only remains to establish (4.23). Applying (4.22) for an upper bound (and using that the first term on the right hand side is non-positive) and the non-magnetic Lieb-Thirring estimate for a lower bound we get

$$\begin{aligned}
CL_0 h^{-1} &\geq \text{Tr} [\chi_u \psi H_h(A=0) \psi \chi_u] - \\
&\geq \frac{1}{2} \text{Tr} [D^2 \tilde{\gamma}_u] + \text{Tr} \left[\frac{1}{2} D^2 - V 1_{\text{supp } \chi_u} \right] - \\
&\geq \frac{1}{2} \text{Tr} [D^2 \tilde{\gamma}_u] - Ch^{-3} \int_{\text{supp } \chi_u} V^{5/2}.
\end{aligned} \quad (4.26)$$

Since $L_0^{-1} \leq Ch^{-1}$ from (4.25) and (3.4), this estimate clearly implies (4.23). This completes the proof of Theorem 3.2. \square

5 Proof of the Semiclassical Theorem 4.1

The rest of the paper is devoted to the proof of the main technical result, Theorem 4.1. We can assume that $f = \ell = 1$ since (4.3) is scale invariant.

For the proof of the upper bound, we just set $A = 0$, i.e.

$$\begin{aligned} \inf'_A \left(\text{Tr} [\psi H_h(A) \psi]_- + \frac{1}{\kappa h^2} \int_{B(2)} |\nabla \otimes A|^2 \right) &\leq \text{Tr} [\psi (D^2 - V) \psi]_- \\ &\leq 2(2\pi h)^{-3} \iint \psi(q)^2 [p^2 - V(q)]_- dq dp + Ch^{-2+1/5}, \end{aligned} \quad (5.1)$$

where the last estimate is a consequence of Theorem 3.3. Actually, the exponent in the error term in the upper bound in (5.1) can be improved from $-2 + 1/5$ to -1 by appealing to Theorem 5.3 below. However, we will not need this.

The proof of the lower bound in Theorem 4.1 has several steps. First, in Section 5.1, we localize onto balls of radius $L_0 \gg h^{1/2}$ at the expense of an acceptable error of order $O(h^{1+\varepsilon})$, in fact we will choose $L_0 := h^{1/2-\varepsilon_0}$ with some small ε_0 , and ε will depend on ε_0 . (Note that here L_0 is chosen differently than in the proof of Theorem 3.2.) Then we wish to replace A by a smoothed out version A_r on scale $r := h^{1/2+\rho} \ll h^{1/2}$ for some small $\rho > 0$ with an error of order $O(h^{1+\varepsilon})$, where ε will depend on ϱ . This will eventually be achieved in Section 5.2 (Theorem 5.2). In order to do that, we will need apriori bounds on the magnetic field and the momentum distribution of the low energy trial states. To obtain these apriori bounds, in Section 6.2 we will introduce a second localization on an intermediate scale $L_1 = h^{1/2+\varepsilon_0}$ with $r \ll L_1 \ll L_0$, and we show that on this scale A can be neglected. These apriori bounds will have a weaker precision of order $O(h^{1-\varepsilon})$ since localization onto a short scale $L_1 \ll h^{1/2}$ is expensive, but this will be sufficient as an input for Section 5.2.

Finally we go back to the larger scale L_0 and use a semiclassical result for the operator with the smoothed vector potential A_r . Note that the scale of regularity, r , of the vector potential is much smaller than L_0 , so it is not a straightforward application of standard semiclassical results with C^∞ data. However, one can keep track of the dependence of the error terms in the standard semiclassical statements on the derivatives of the symbol, which in our case will be powers of L_0/r . If L_0/r is not too large, this error can be compensated by the smallness of A , still rendering a few derivatives of A_r bounded which is sufficient for the semiclassical asymptotics.

5.1 Localization onto balls of size L_0

We introduce a partition of unity on the lengthscale $L_0 = h^{1/2-\varepsilon_0} \leq 1/4$ with some sufficiently small $\varepsilon_0 > 0$, i.e. we choose $\phi_* \in C_0^\infty(\mathbb{R}^3)$, $\int \phi_*^2 = 1$, $\text{supp } \phi_* \subset B(1)$, and define

$$\phi_u(x) = \phi_*\left(\frac{x-u}{L_0}\right)$$

then

$$\int_{\mathbb{R}^3} \phi_u^2(x) \frac{du}{L_0^3} \equiv 1.$$

Inserting this identity into $\text{Tr} [\psi H_h(A) \psi]_-$ and using IMS localization, we have

$$\begin{aligned} \text{Tr} [\psi H_h(A) \psi]_- &= \text{Tr} \left[\int_{B(3/2)} \frac{du}{L_0^3} \psi \left[\phi_u H_h(A) \phi_u - h^2 |\nabla \phi_u|^2 \right] \psi \right]_- \\ &\geq \text{Tr} \left[\int_{B(3/2)} \frac{du}{L_0^3} \psi \phi_u (H_h(A) - Ch^2 L_0^{-2}) \phi_u \psi \right]_- \geq \int_{B(3/2)} \frac{du}{L_0^3} \text{Tr} \left[\psi \phi_u (H_h(A) - Ch^2 L_0^{-2}) \phi_u \psi \right]_- \end{aligned}$$

after reallocating the localization error. Notice that the du integration can be restricted to $B(3/2)$, otherwise $\psi \phi_u = 0$. We can again redefine the potential

$$V \rightarrow V^+ := V + Ch^2 L_0^{-2}.$$

The change of the semiclassical term due to this modification,

$$\begin{aligned} &\left| 2(2\pi h)^{-3} \iint \psi(q)^2 [p^2 - V(q)]_- dq dp - 2(2\pi h)^{-3} \iint \psi(q)^2 [p^2 - V^+(q)]_- dq dp \right| \\ &\leq Ch^{-3} h^2 L_0^{-2} \leq Ch^{-2+2\varepsilon_0}, \quad (5.2) \end{aligned}$$

can be incorporated into the error term in (4.3). Therefore to prove the lower bound in (4.3), it is sufficient to prove that, for some $\varepsilon > 0$,

$$\begin{aligned} \inf_A' \left(\int_{B(3/2)} \frac{du}{L_0^3} \text{Tr} [\psi \phi_u H_h^+(A) \phi_u \psi]_- + \frac{1}{\kappa h^2} \int_{B(2)} |\nabla \otimes A|^2 \right) \\ \geq 2(2\pi h)^{-3} \iint \psi(q)^2 [p^2 - V^+(q)]_- dq dp - Ch^{-2+\varepsilon}, \quad (5.3) \end{aligned}$$

where $H_h^+ := T_h - V^+$. Since V^+ satisfies the same bound as V (second bound in (4.1) with $f = \ell = 1$), we can drop the upper index $+$ and we will focus on the proof of (5.3).

We reallocate the magnetic energy and consider the infimum over A for each u separately. Reallocation changes the coefficient of the field energy by a universal constant factor $c > 0$ using the inequality

$$\int_{B(2)} |\nabla \otimes A|^2 \geq c \int_{B(3/2)} \frac{du}{L_0^3} \int_{B_u(2L_0)} |\nabla \otimes A|^2.$$

Therefore, it is sufficient to prove that for each fixed $u \in B(3/2)$ and $c > 0$ we have

$$\begin{aligned} \inf_A' \left(\text{Tr} [\psi \phi_u H_h(A) \phi_u \psi]_- + \frac{c}{\kappa h^2} \int_{B_u(2L_0)} |\nabla \otimes A|^2 \right) \\ \geq 2(2\pi h)^{-3} \iint \psi(q)^2 \phi_u^2 [p^2 - V(q)]_- dq dp - Ch^{-2+\varepsilon} L_0^3, \quad (5.4) \end{aligned}$$

and then integrating this inequality w.r.t. du/L_0^3 over $u \in B(3/2)$, we will obtain (5.3). Recall that \inf'_A denotes infimum over vector potentials with $\nabla \cdot A = 0$ on $B(5/4)$, in particular they are divergence free in a neighborhood of the support of ψ .

Defining $\phi = \psi\phi_u$, Theorem 4.1 will immediately follow from the following theorem

Theorem 5.1. *Let $L_0 = h^{1/2-\varepsilon_0}$ with a sufficiently small $\varepsilon_0 > 0$. Let ϕ be supported in $B(L_0)$, with $|\partial^n \phi| \leq C_n L_0^{-|n|}$. Let the potential V satisfy*

$$|\partial^n V| \leq C_n \quad \text{on } \overline{B}(L_0), \quad \text{and} \quad V(0) \geq c_0 \quad (5.5)$$

with some positive constants C_n and c_0 . Then for any $\kappa > 0$ we have

$$\begin{aligned} \inf'_A \left(\text{Tr} [\phi H_h(A) \phi]_- + \frac{1}{\kappa h^2} \int_{B(2L_0)} |\nabla \otimes A|^2 \right) \\ \geq 2(2\pi h)^{-3} \iint \phi(q)^2 [p^2 - V(q)]_- dq dp - Ch^{1+\varepsilon_0} \Lambda_{L_0} \end{aligned} \quad (5.6)$$

with a constant C depending on κ , C_n and c_0 , where we recall $\Lambda_{L_0} = h^{-3} L_0^3$. Here \inf'_A is taken for all vector potentials satisfying $\nabla \cdot A = 0$ on $B(5L_0/4)$.

In the next subsections of Section 5 we will prove Theorem 5.1. We first smooth out the magnetic vector potential, A , on a scale $r \ll h^{1/2}$. Theorem 5.2 in Section 5.2 states that the error of this replacement is negligible. This is the main technical result and it will be proven in Section 6. Once A is replaced with a smoothed version A_r , and we estimate the size of its derivatives, we can apply a semiclassical result (Theorem 5.3) to evaluate the r.h.s. of (5.11). Combining Theorem 5.2 and Theorem 5.3 will then yield Theorem 5.1.

5.2 Replacing A with a smooth version on L_0 -box

To prove Theorem 5.1, we first smooth out the magnetic potential on a scale $r = h^{1/2+\varepsilon} \ll h^{1/2}$. Using the lower bound from Theorem 3.3, it is sufficient to consider magnetic vector potentials A such that

$$\mathcal{E}(A) := \text{Tr} [\phi H_h(A) \phi]_- + \frac{1}{\kappa h^2} \int_{B(2L_0)} |\nabla \otimes A|^2 \leq \mathcal{E}(0).$$

We can assume that A has zero average, i.e.

$$\int_{B(2L_0)} A = 0, \quad (5.7)$$

since $\mathcal{E}(A) = \mathcal{E}(A - c)$ for any constant shift $c \in \mathbb{R}^3$ in the vector potential. To see this, note that for any cutoff function ψ , by the variational principle,

$$\begin{aligned} \text{Tr} [\psi(T_h(A) - V)\psi]_- &= \inf \{ \text{Tr} \psi(T_h(A) - V)\psi\gamma : 0 \leq \gamma \leq 1 \} \\ &= \inf \{ \text{Tr} \psi(T_h(A - c) - V)\psi e^{-ic \cdot x/h} \gamma e^{ic \cdot x/h} : 0 \leq \gamma \leq 1 \} \\ &= \inf \{ \text{Tr} \psi(T_h(A - c) - V)\psi\gamma : 0 \leq \gamma \leq 1 \} \\ &= \text{Tr} [\psi(T_h(A - c) - V)\psi]_-. \end{aligned} \quad (5.8)$$

In fact, $\text{Tr} [\psi(T_h(A) - V)\psi]_-$ is invariant under any gauge transformation, $A \rightarrow A - \nabla\varphi$, $\varphi : \mathbb{R}^3 \rightarrow \mathbb{R}$, but $\int_{B(2L_0)} |\nabla \otimes A|^2$ is not.

Now we state the main result of this section:

Theorem 5.2. *Let $\kappa > 0$ be given. Let $L_0 = h^{1/2-\varepsilon_0}$ for some sufficiently small $\varepsilon_0 > 0$. Let ϕ with $\text{supp } \phi \subset B(L_0)$ with $|\partial^n \phi| \leq C_n L_0^{-|n|}$. Assume that the potential V satisfies*

$$|\partial^n V| \leq C_n \quad \text{on } \overline{B}(L_0) \quad \text{and} \quad V(0) \geq c_0 \quad (5.9)$$

with some positive constants C_n and c_0 . Let A be a vector potential such that $\mathcal{E}(A) \leq \mathcal{E}(0)$ and satisfying (5.7) and $\nabla \cdot A = 0$ on $B(5L_0/4)$. Then for $\alpha := 1 - 3\varepsilon_0$ we have

$$h^{-2} \int_{B(2L_0)} |\nabla \otimes A|^2 \leq Ch^\alpha \Lambda_{L_0}. \quad (5.10)$$

Moreover, for $\rho > 0$ sufficiently small there exists $\varepsilon_0 > 0$ (in the definition of L_0) such that with $r := h^{1/2+\rho}$ we have

$$\text{Tr} (\phi[T_h(A) - V]\phi)_- + \frac{1}{\kappa h^2} \int_{B(2L_0)} |\nabla \otimes A|^2 \geq \text{Tr} (\phi[T_h(A_r) - V]\phi)_- - Ch^{1+\varepsilon_0} \Lambda_{L_0}. \quad (5.11)$$

*Here $A_r = A * \chi_r$ is a smoothed out version of A on the length scale r and the constants in the estimates depend on the fixed unscaled cutoff function χ , on κ , C_n and c_0 in (5.9).*

We remark that this theorem involves only the potential in $B(L_0)$. However, under the conditions (5.9) one can extend V to $\overline{B}(2L_0)$ with similar bounds on the derivative. In the sequel we will thus assume that V is defined in $B(2L_0)$ with

$$|\partial^n V| \leq C_n \quad \text{on } \overline{B}(2L_0) \quad \text{and} \quad V(0) \geq c_0, \quad (5.12)$$

for some constants C_n and c_0 that is determined by, but may differ from, the constants in (5.9) and with a slight abuse of notations we will continue to use the same letters.

Theorem 5.2 will be proved in Section 6 below.

5.3 A precise semiclassical result

We state the following simplified version of [I, Theorem 4.5.2] (see also [I2, Theorem 5.2.2]) for reference. Recall that $D = -ih\nabla$.

Theorem 5.3. *Suppose that ϕ is a localization function with*

$$\text{supp } \phi \subset B(1), \quad (5.13)$$

and $H = (D + A)^2 - V$ is a self-adjoint magnetic Schrödinger operator acting on $L^2(\mathbb{R}^3)$ with

$$|\partial^n V| \leq c, \quad |\partial^n A| \leq c, \quad \text{and} \quad |\partial^n \phi| \leq c \quad (5.14)$$

for all multi-indices $n \in \mathbb{N}^3$ with $|n| \leq K$. Then, for all $h \in (0, 1]$,

$$\left| \text{Tr}_{L^2(\mathbb{R}^3)} \phi^2 [(D + A)^2 - V]_- - (2\pi h)^{-3} \iint \phi^2(q) [(p + A(q))^2 - V(q)]_- \, dq dp \right| \leq Ch^{-1}. \quad (5.15)$$

Here K is a universal constant and C only depends on the constant c in (5.14).

The same result holds for the Pauli operator $T_h(A) = [\boldsymbol{\sigma} \cdot (D + A)]^2$ as well

$$\left| \text{Tr } \phi^2 [T_h(A) - V]_- - 2(2\pi h)^{-3} \iint \phi^2(q) [(p + A(q))^2 - V(q)]_- \, dq dp \right| \leq Ch^{-1}. \quad (5.16)$$

Remark 5.4. *By a simple shift of variables $p \rightarrow p + A(q)$ for each fixed q , we obtain that*

$$(2\pi h)^{-3} \iint \phi^2(q) [(p + A(q))^2 - V(q)]_- \, dq dp = (2\pi h)^{-3} \iint \phi^2(q) [p^2 - V(q)]_- \, dq dp,$$

in other words, the presence of the magnetic vector potential plays no role in the semiclassical formula.

Remark 5.5. *Theorem 5.3 in Ivrii's book is formulated for Schrödinger operators, as stated in (5.15) above. For the purpose of semiclassical analysis, the Pauli operator, written as $T_h(A) = (D + A)^2 + h\boldsymbol{\sigma} \cdot B - V$, can be considered as a Schrödinger operator with 2×2 matrix valued potential that is subprincipal. Therefore the analysis of Ivrii goes through for the Pauli case as well and this gives (5.16). Alternatively, one can apply Ivrii's result for the Dirac operator [I, Theorem 7.3.14] or [I2, Theorem 5.2.23] and use that in the large mass m limit, the square of the Dirac operator converges to the Pauli operator. Although not stated explicitly, the error estimates in the cited theorems are uniform as $m \rightarrow \infty$. In this way, taking the semiclassical limit followed by the large mass limit, the semiclassical estimate for the Pauli operator can be deduced from Ivrii's result on the Dirac operator.*

We also need a slight modification of Theorem 5.3 when the localization function ϕ is inside the negative part:

Theorem 5.6. Suppose that ϕ is a localization function with

$$\text{supp } \phi \subset B(1), \quad (5.17)$$

and $H = T_h(A) - V$ is a self-adjoint Pauli operator acting on $L^2(\mathbb{R}^3, \mathbb{C}^2)$ with

$$|\partial^n V| \leq c, \quad |\partial^n A| \leq c, \quad \text{and} \quad |\partial^n \phi| \leq c \quad (5.18)$$

for all multi-indices $n \in \mathbb{N}^3$ with $|n| \leq K$. Then, for all $h > 0$,

$$\left| \text{Tr} [\phi(T_h(A) - V)\phi]_- - 2(2\pi h)^{-3} \iint \phi^2(q) [p^2 - V(q)]_- dq dp \right| \leq Ch^{-1}. \quad (5.19)$$

Here K is a universal constant and C only depends on the constant c in (5.18). Similar statement holds for the magnetic Schrödinger operator.

Proof. Since this estimate is local, we may assume that $\text{supp } V, \text{supp } A \subseteq B(2)$. For a lower bound we estimate

$$\text{Tr} [\phi(T_h(A) - V)\phi]_- \geq \text{Tr} [\phi(T_h(A) - V)_- \phi]_- = \text{Tr} [\phi(T_h(A) - V)_- \phi]. \quad (5.20)$$

In order to prove the upper bound, we write $\gamma := \mathbf{1}_{(-\infty, 0]}(H)$ and calculate,

$$\begin{aligned} \text{Tr } \phi^2[H]_- &= \frac{1}{2} \text{Tr} (\phi^2[H]_- + [H]_- \phi^2) = \frac{1}{2} \text{Tr} ((\phi^2 H + H \phi^2) \gamma) \\ &= \frac{1}{2} \text{Tr} (([H, \phi], \phi) + 2\phi H \phi) \gamma. \end{aligned} \quad (5.21)$$

Therefore, by the variational principle,

$$\text{Tr} [\phi H \phi]_- \leq \text{Tr } \phi^2[H]_- + h^2 \text{Tr} (\nabla \phi)^2 \gamma. \quad (5.22)$$

In order to estimate the last term we apply a Lieb-Thirring inequality to the operator $H - (\nabla \phi)^2$. Using $\text{Tr } H \gamma \leq 0$, this yields

$$\begin{aligned} -\text{Tr} (\nabla \phi)^2 \gamma &\geq \text{Tr} (H - (\nabla \phi)^2) \gamma \\ &\geq -Ch^{-3} \int ([V]_+ + (\nabla \phi)^2)^{5/2} - C \left(h^{-2} \int |\nabla \times A|^2 \right)^{3/4} \left(\int ([V]_+ + (\nabla \phi)^2)^4 \right)^{1/4} \\ &\geq -Ch^{-3} - Ch^{-3/2}. \end{aligned} \quad (5.23)$$

For Schrödinger a similar Lieb-Thirring inequality holds but without the magnetic term.

Combining the upper and lower bounds the estimate (5.19) follows from (5.15) in case of $h \leq 1$. Finally, for $h \geq 1$ (5.19) trivially holds since the semiclassical integral is of order h^{-3} which is smaller than Ch^{-1} . The quantum energy can be bounded by the Lieb-Thirring inequality after using (5.20):

$$0 \geq \text{Tr} [\phi(T_h(A) - V)\phi]_- \geq \text{Tr} (T_h(A) - V)_- \geq -Ch^{-3} - Ch^{-3/2}$$

for the Pauli case and the $h^{-3/2}$ term is absent for the Schrödinger case. Both terms are smaller than the error bar Ch^{-1} in (5.19). \square

Now we explain how Theorem 5.3 can be applied to prove Theorem 5.1 from Theorem 5.2.

To estimate the right hand side of (5.11) from below, we first move the localization outside the negative part by the simple inequality

$$\mathrm{Tr} \left(\phi[(T_h(A_r) - V)\phi]_- \right) \geq \mathrm{Tr} \phi[T_h(A_r) - V]_- \phi = \mathrm{Tr} \phi^2[T_h(A_r) - V]_-. \quad (5.24)$$

By unitary scaling $x \rightarrow L_0 x$, we scale the unit ball to the ball $B(L_0)$ and we have

$$\mathrm{Tr} \phi^2[T_h(A_r) - V]_- = \mathrm{Tr} \tilde{\phi}^2[T_{h/L_0}(\tilde{A}_r) - \tilde{V}]_-, \quad (5.25)$$

where

$$\tilde{\phi}(x) = \phi(L_0 x), \quad \mathrm{supp} \tilde{\phi} \subset B(1), \quad (5.26)$$

and

$$\tilde{V}(x) = V(L_0 x), \quad \tilde{A}_r(x) = A_r(L_0 x). \quad (5.27)$$

Notice that the semiclassical parameter has changed from h to $h_{new} := h/L_0 = h^{\frac{1}{2} + \varepsilon_0}$ which is much smaller than $h^{1/2}$. Theorem 5.3 will be used for the data with tilde with h_{new} and it provides a precise semiclassical asymptotics with a relative error term of order Ch_{new}^2 compared with the main term. In terms of the original h , this error is of order $Ch^{1+2\varepsilon_0}$.

We now check that the derivative estimates (5.14) hold for \tilde{V} , \tilde{A}_r and $\tilde{\phi}$. Notice that we may replace V and A_r by localized versions in the left hand side of (5.24). Therefore, we only need to control the (finitely many) derivatives in (5.14) in the ball $B(3/2)$.

Clearly, the derivatives of $\tilde{\phi}$ and \tilde{V} are bounded since $L_0 \leq 1$. For \tilde{A}_r we have the following estimate which will be proved as a consequence of Lemma 6.16 in Section 6.3.

Lemma 5.7. *Assume that $\int_{B(2L_0)} A = 0$, then the following estimate holds, for $|n| \geq 0$,*

$$\int_{B(3/2)} |\partial^n \tilde{A}_r|^2 \leq C_n \left(\frac{L_0}{r} \right)^{2 \max(|n|-1, 0)} L_0^{-1} \int_{B(2L_0)} |\nabla \otimes A|^2. \quad (5.28)$$

Lemma 5.7 combined with (5.10), yield

$$\int_{B(3/2)} |\partial^n \tilde{A}_r|^2 \leq C \left(\frac{L_0}{r} \right)^{2 \max(|n|-1, 0)} L_0^2 h^{\alpha-1}. \quad (5.29)$$

In order to use Theorem 5.3 we need uniform bounds on K derivatives of \tilde{A}_r . By Sobolev inequalities this corresponds to $K' > K + 3/2$ L^2 -derivatives. Inserting $|n| = K'$ and the definitions of L_0, r and α in (5.29), we get

$$\int_{B(3/2)} |\partial^n \tilde{A}_r|^2 \leq Ch^{1-2(K'-1)\rho-(2K'+2)\varepsilon_0}, \quad (5.30)$$

for all $n \in \mathbf{N}^3$ with $|n| \leq K'$. Since K' is universal, the right side of (5.30) is clearly bounded for sufficiently small ρ and ε_0 , i.e. if

$$1 \geq (2K' - 2)\rho - (2K' + 2)\varepsilon_0. \quad (5.31)$$

By Theorem 5.3, applied to the Pauli operator, we get for such values of ρ, ε_0 that

$$\begin{aligned} \text{Tr } \tilde{\phi}^2 [T_{h/L_0}(\tilde{A}_r) - \tilde{V}]_- &= 2(2\pi(h/L_0))^{-3} \iint \tilde{\phi}^2(q) [(p + \tilde{A}_r(q))^2 - \tilde{V}(q)]_- \, dq dp + \mathcal{O}((h/L_0)^{-1}) \\ &= 2(2\pi h)^{-3} \iint \phi^2(q) [p^2 - V(q)]_- \, dq dp + \mathcal{O}(h^{1+2\varepsilon_0} \Lambda_{L_0}). \end{aligned} \quad (5.32)$$

Recalling that the error in (5.11) was $\mathcal{O}(h^{1+\varepsilon_0} \Lambda_{L_0})$ this completes the proof of Theorem 5.1. \square

6 Proof of Theorem 5.2

6.1 Reduction to a constant potential

We use the notations and assumptions of Theorem 5.2, the extension of V given in (5.12), and assume that $\mathcal{E}(A) \leq \mathcal{E}(0)$. From (5.12) we can assume $V \geq 0$ for h sufficiently small. Let χ be a nonnegative, smooth, symmetric, cutoff function on \mathbb{R}^3 with $\int \chi^2 = 1$ and $\text{supp } \chi \subset B(1)$. We choose a new lengthscale $L_1 \leq \frac{1}{4}L_0$ such that $h \leq L_1 \leq h^{1/2} |\log h|^{-2}$. For any $u \in \mathbb{R}^3$ we denote

$$\chi_u(x) = \chi_{u, L_1}(x) = \chi\left(\frac{x - u}{L_1}\right), \quad \int \frac{du}{L_1^3} \chi_u^2(x) \equiv 1, \quad (6.1)$$

and we will mostly omit the lengthscale L_1 . In the applications, $L_1 = h^{1/2+\varepsilon_0}$.

We first prove a rough lower bound on the left hand side of (5.11). This will eventually be used to get apriori bounds when we prove (5.11). Along the way, we also prove (5.10).

Theorem 6.1. *Fix $\kappa > 0$ and assume that the potential satisfies (5.9). Let $\phi \in C_0^\infty(B(L_0))$ with $|\partial^n \phi| \leq C_n L_0^{-|n|}$ and let A be a vector potential satisfying (5.7) and $\nabla \cdot A = 0$ on $B(5L_0/4)$. For any $\alpha < 1$ and $\delta > 0$ there is a constant $C_{\delta, \alpha}$ such that if $h \leq h_\delta$, then*

$$\begin{aligned} \text{Tr } [\phi [T_h(A) - V] \phi]_- &+ \frac{1}{\kappa h^2} \int_{B(2L_0)} |\nabla \otimes A|^2 \\ &\geq \int \text{Tr } \left[\chi_u \phi [D^2 - V(u)]_- \phi \chi_u \right] \frac{du}{L_1^3} + (\kappa^{-1} - C\delta) h^{-2} \int_{B(2L_0)} |\nabla \otimes A|^2 \\ &\quad - \left(C_{\delta, \alpha} h^\alpha + C h^2 L_1^{-2} + C L_1^2 \right) \Lambda_{L_0}. \end{aligned} \quad (6.2)$$

Moreover, we also have

$$\begin{aligned} \inf_A \left\{ \text{Tr} \left[\phi [T_h(A) - V] \phi \right]_- + \frac{1}{\kappa h^2} \int_{B(2L_0)} |\nabla \otimes A|^2 \right\} \\ \leq \int \text{Tr} \left[\chi_u \phi [D^2 - V(u)]_- \phi \chi_u \right] \frac{du}{L_1^3} + C(h^2 L_1^{-2} + L_1^2) \Lambda_{L_0}. \end{aligned} \quad (6.3)$$

Remark 6.2. We have explicitly, for any $u \in \mathbb{R}^3$,

$$\text{Tr} \left[\chi_u \phi [D^2 - V(u)]_- \phi \chi_u \right] = -\frac{2}{15\pi^2} h^{-3} [V(u)]^{5/2} \int \phi^2 \chi_u^2$$

and thus

$$\int \text{Tr} \left[\chi_u \phi [D^2 - V(u)]_- \phi \chi_u \right] du = -\frac{2}{15\pi^2} h^{-3} \int \int [V(u)]^{5/2} \chi_u^2(x) \phi(x) dx du.$$

After expansion

$$[V(u)]^{5/2} = [V(x)]^{5/2} + \nabla[V(x)]^{5/2}(x - u) + O([x - u]^2)$$

and since, for any $x \in \mathbb{R}^3$,

$$\int du \chi_u^2(x)(x - u) = 0$$

by symmetry, so we have

$$\int \text{Tr} \left[\chi_u \phi [D^2 - V(u)]_- \phi \chi_u \right] \frac{du}{L_1^3} = -\frac{2}{15\pi^2} h^{-3} \int V^{5/2} \phi^2 + O(L_1^2 h^{-3}) \int \phi^2. \quad (6.4)$$

Moreover, we have the following upper bound on the magnetic energy:

Corollary 6.3. Under the conditions of Theorem 5.2 we have

$$\frac{1}{2\kappa h^2} \int_{B(2L_0)} |\nabla \otimes A|^2 \leq \left(C_{\delta, \alpha} h^\alpha + C h^2 L_1^{-2} + C L_1^2 \right) \Lambda_{L_0}$$

for all sufficiently small h .

Corollary 6.3 is an immediate consequence of (6.2) from Theorem 6.1 choosing δ sufficiently small, using $\mathcal{E}(A) \leq \mathcal{E}(0)$ and Theorem 5.6 (with rescaling it to the ball of size L_0). Choosing $L_1 = h^{1/2+\varepsilon_0}$ and $\alpha = 1 - 3\varepsilon_0$, we immediately obtain (5.10), the first claim of Theorem 5.2.

Proof of Theorem 6.1. First we give the lower bound (6.2). Recall that we can extend the potential V from $\overline{B}(L_0)$ to $B(2L_0)$ by keeping similar derivative bounds as in (5.9), see (5.12). By the IMS formula, and Taylor expansion

$$\left| V(x) - V(u) - \nabla V(x) \cdot (x - u) \right| \leq C(x - u)^2 \quad (6.5)$$

for all $x \in \text{supp } \phi$, $u \in \text{supp } \phi + L_1 \text{supp } \chi$, we have

$$\begin{aligned}
\phi[T_h(A) - V]\phi &= \int \chi_u^2(x)\phi(x)[T_h(A) - V(x)]\phi(x)\frac{du}{L_1^3} \\
&\geq \int \chi_u(x)\phi(x)\left[T_h(A) - V(x) - Ch^2L_1^{-2}\right]\phi(x)\chi_u(x)\frac{du}{L_1^3} \\
&\geq \int \chi_u(x)\phi(x)\left[T_h(A) - V(u) - \nabla V(x) \cdot (x - u) - Ch^2L_1^{-2} - CL_1^2\right]\phi(x)\chi_u(x)\frac{du}{L_1^3} \\
&= \int \chi_u(x)\phi(x)\left[T_h(A) - V(u) - Ch^2L_1^{-2} - CL_1^2\right]\phi(x)\chi_u(x)\frac{du}{L_1^3}. \tag{6.6}
\end{aligned}$$

In the last step we used that

$$\int (x - u)\chi_u^2(x)du = 0. \tag{6.7}$$

Using that $\text{Tr } [\sum_j A_j]_- \geq \sum_j \text{Tr } [A_j]_-$, we get

$$\text{Tr } [\phi[T_h(A) - V]\phi]_- \geq \int \text{Tr } [\chi_u\phi[T_h(A) - V(u) - Ch^2L_1^{-2} - CL_1^2]\phi\chi_u]_- \frac{du}{L_1^3}. \tag{6.8}$$

In Theorem 6.4 of the next section, we will prove that A can be neglected. In order to facilitate the estimate, it is convenient to ensure that A has zero average on the ball $B_u(2L_1)$. We define

$$c_u := \int_{B_u(2L_1)} A. \tag{6.9}$$

Similarly to the argument in (5.8), we can subtract c_u from A in (6.8) and we have

$$\text{Tr } [\phi[T_h(A) - V]\phi]_- \geq \int \text{Tr } [\chi_u\phi[T_h(A - c_u) - V(u) - Ch^2L_1^{-2} - CL_1^2]\phi\chi_u]_- \frac{du}{L_1^3}. \tag{6.10}$$

The u -integration in (6.10) can be restricted to $u \in B(\frac{5}{4}L_0)$ by the support properties of ϕ and χ_u . For each fixed $u \in B(\frac{5}{4}L_0)$ we will use Theorem 6.4 proven in the next section to estimate the trace in the integrand. Define

$$V_u := V(u) + Ch^2L_1^{-2} + CL_1^2. \tag{6.11}$$

By (5.12) we know that $c_0/2 \leq V_u \leq C$. With the choice of $L = L_1$, $W = V_u$ and $\eta = \chi_u\phi$, we see from Theorem 6.4 that for any $\alpha < 1$, $\varepsilon > 0$ and for any $\delta > 0$ there is a constant $C_{\delta,\varepsilon}$ such that

$$\begin{aligned}
&\text{Tr } [\chi_u\phi[T_h(A - c_u) - V(u) - Ch^2L_1^{-2} - CL_1^2]\phi\chi_u]_- \\
&\geq \text{Tr } \chi_u\phi[D^2 - V_u]_- \phi\chi_u - \delta V_u^{1/2}h^{-2} \int_{B_u(2L_1)} |\nabla \otimes A|^2 - C_{\delta,\varepsilon}h^\alpha V_u^{5/2}\Lambda_{L_1} \tag{6.12}
\end{aligned}$$

as long as

$$h^{1-\frac{\alpha}{2}-\varepsilon}V_u^{-1/2} \leq L_1 \leq Ch^{1/2}|\log h|^{-2}V_u^{-1/2} \quad (6.13)$$

and

$$h^{-2} \int_{B_u(2L_1)} |\nabla \otimes A|^2 \leq C\Lambda_{L_1} V_u^2 \quad (6.14)$$

hold for some constant C . The constant $C_{\delta,\varepsilon}$ will also depend on the constants in (6.13) and (6.14).

Recalling $L_1 = h^{1/2+\varepsilon_0}$, with the choice $\alpha = 1 - 3\varepsilon_0$ and $\varepsilon < \varepsilon_0/2$, we see that (6.13) is always satisfied since $c_0/2 \leq V_u \leq C$ uniformly in $u \in B(2L_0)$. To guarantee the second condition (6.14) for the availability of the estimate (6.12), we split the integral on the r.h.s. of (6.10) as follows

$$\int_{B(5L_0/4)} \text{Tr} [\dots]_- \frac{du}{L_1^3} = \int \mathbf{1}\{u \in \Xi_{<}\} \text{Tr} [\dots]_- \frac{du}{L_1^3} + \int \mathbf{1}\{u \in \Xi_{>}\} \text{Tr} [\dots]_- \frac{du}{L_1^3}, \quad (6.15)$$

where we defined

$$\begin{aligned} \Xi_{<} &:= \left\{ u \in B\left(\frac{5}{4}L_0\right) : \delta h^{-2} \int_{B_u(2L_1)} |\nabla \otimes A|^2 \leq \Lambda_{L_1} V_u^2 \right\} \\ \Xi_{>} &:= \left\{ u \in B\left(\frac{5}{4}L_0\right) : \delta h^{-2} \int_{B_u(2L_1)} |\nabla \otimes A|^2 \geq \Lambda_{L_1} V_u^2 \right\}. \end{aligned}$$

The estimate (6.12) will thus be available for u 's in the first integral and it yields

$$\begin{aligned} &\int \mathbf{1}\{u \in \Xi_{<}\} \text{Tr} \left[\chi_u \phi [T_h(A - c_u) - V(u) - Ch^2 L_1^{-2} - CL_1^2] \phi \chi_u \right]_- \frac{du}{L_1^3} \\ &\geq \int \mathbf{1}\{u \in \Xi_{<}\} \left(\text{Tr} \chi_u \phi [D^2 - V_u]_- \phi \chi_u \right) \frac{du}{L_1^3} - C\delta h^{-2} \int_{B(2L_0)} |\nabla \otimes A|^2 - C_{\delta,\alpha} h^\alpha \Lambda_{L_1}. \end{aligned} \quad (6.16)$$

With an explicit calculation, for any $\beta > 0$ constant and cutoff function η , we have

$$\text{Tr} \eta [D^2 - \beta]_- \eta = 2(2\pi)^{-3} \int \eta^2(x) dx \int [(hp)^2 - \beta]_- dp = \frac{2}{15\pi^2} h^{-3} \beta^{5/2} \int \eta^2$$

(the additional factor 2 comes from the spin degeneracy). Since $|V(u)| \leq C$, $h \leq L_1 \leq 1$ and $V_u > 0$, we obtain

$$V_u^{5/2} \leq [V(u)]_+^{5/2} + C(h^2 L_1^{-2} + L_1^2), \quad (6.17)$$

and thus

$$\text{Tr} \chi_u \phi [D^2 - V_u]_- \phi \chi_u \geq \text{Tr} \chi_u \phi [D^2 - V(u)]_- \phi \chi_u - C(h^2 L_1^{-2} + L_1^2) \Lambda_{L_1}.$$

Inserting this into (6.16), we have the following estimate for the first integral on the r.h.s. of (6.15):

$$\begin{aligned} \int \mathbf{1}\{u \in \Xi_{<}\} [\dots] \frac{du}{L_1^3} &\geq \int \mathbf{1}\{u \in \Xi_{<}\} \left(\text{Tr } \chi_u \phi [D^2 - V(u)]_- \phi \chi_u \right) \frac{du}{L_1^3} \\ &\quad - C\delta h^{-2} \int_{B(2L_0)} |\nabla \otimes A|^2 - [C_{\delta,\alpha} h^\alpha + Ch^2 L_1^{-2} + CL_1^2] \Lambda_{L_1}. \end{aligned} \quad (6.18)$$

The traces in the second integral of (6.15) are directly estimated using a Lieb-Thirring bound. For this estimate we will have to localize the magnetic field. Fix $u \in \Xi_{>}$ and choose a cutoff function ϕ' with $\text{supp } \phi' \subset B_u(3L_1/2)$, $|\partial^n \phi'| \leq C_n L_1^{-n}$ and such that $\phi' \equiv 1$ on $B(L_1)$ and define, for the purpose of this proof,

$$A' = (A - c_u)\phi', \quad V'(x) = V_u \cdot \mathbf{1}\{x \in B_u(L_1)\}. \quad (6.19)$$

Clearly

$$\int_{\mathbb{R}^3} |\nabla \otimes A'|^2 \leq \int_{B_u(2L_1)} |\nabla \otimes A|^2 + CL_1^{-2} \int_{B_u(2L_1)} |A - c_u|^2 \leq C \int_{B_u(2L_1)} |\nabla \otimes A|^2 \quad (6.20)$$

where in the second step we used the Poincaré inequality.

By the magnetic Lieb-Thirring inequality, Theorem 2.4, and (6.20):

$$\begin{aligned} \text{Tr } [\chi_u \phi [T_h(A - c_u) - V(u) - Ch^2 L_1^{-2} - CL_1^2] \phi \chi_u]_- &= \text{Tr } [\chi_u \phi [T_h(A') - V'] \phi \chi_u]_- \\ &\geq -Ch^{-3} \int_{B_u(L_1)} V_u^{5/2} - C \left(h^{-2} \int_{\mathbb{R}^3} |\nabla \times A'|^2 \right)^{3/4} \left(\int_{B_u(L_1)} V_u^4 \right)^{1/4} \\ &\geq -\delta h^{-2} \int_{B_u(2L_1)} |\nabla \otimes A|^2 - C(V_u^{5/2} + h^3 \delta^{-3} V_u^4) \Lambda_{L_1} \\ &\geq -C\delta h^{-2} \int_{B_u(2L_1)} |\nabla \otimes A|^2, \end{aligned} \quad (6.21)$$

using that $V_u \leq C$ and $h \leq h_\delta$. In the last step we used $u \in \Xi_{>}$ to estimate $V_u^2 \Lambda_{L_1}$ by the local magnetic field energy. Integrating out this inequality for $u \in B(5L_0/4)$, we obtain the following bound for the second integral on the r.h.s in (6.15)

$$\int \mathbf{1}\{u \in \Xi_{>}\} [\dots] \frac{du}{L_1^3} \geq -C\delta h^{-2} \int_{B(2L_0)} |\nabla \otimes A|^2. \quad (6.22)$$

Finally, the missing piece of the non-magnetic term on the r.h.s of (6.18) for $u \in \Xi_{>}$ can be estimated by the standard Lieb-Thirring similarly to (6.21) and (6.22)

$$\int \mathbf{1}(u \in \Xi_{>}) \text{Tr } [\chi_u \phi [D^2 - V_u] \phi \chi_u]_- \frac{du}{L_1^3} \geq -C\delta h^{-2} \int_{B_u(2L_0)} |\nabla \otimes A|^2. \quad (6.23)$$

The estimates (6.18), (6.22) and (6.23) inserted into (6.15) and (6.10) complete the proof of (6.2).

For the proof of (6.3), we define the spectral projection

$$\gamma_u := \mathbf{1}_{(-\infty, 0]}(D^2 - V(u) + C(h^2 L_1^{-2} + L_1^2))$$

and

$$\gamma := \int \chi_u \gamma_u \chi_u \frac{du}{L_1^3}.$$

Note that $0 \leq \gamma \leq 1$ by (6.1). We will also use that the density of γ_u is given by

$$\varrho_{\gamma_u}(x) := \gamma_u(x, x) = \frac{4\pi}{3} h^{-3} [V(u) - C(h^2 L_1^{-2} + L_1^2)]_+^{3/2}.$$

Then, by Taylor expanding V up to second order, similarly as in (6.5) but using $\nabla V(u)$ instead of $\nabla V(x)$, we have

$$\begin{aligned} \inf_A \left\{ \text{Tr} \left[\phi [T_h(A) - V] \phi \right]_- + \frac{1}{\kappa h^2} \int |\nabla \otimes A|^2 \right\} &\leq \text{Tr} \left[\phi [D^2 - V] \phi \right]_- \\ &\leq \text{Tr} \phi [D^2 - V] \phi \gamma \\ &= \int \text{Tr} \left(\chi_u \phi [D^2 - V] \phi \chi_u \gamma_u \right) \frac{du}{L_1^3} \\ &\leq \int \text{Tr} \left(\chi_u \phi [D^2 - V(u) - \nabla V(u) \cdot (x - u) + C L_1^2] \phi \chi_u \gamma_u \right) \frac{du}{L_1^3} \\ &= \int \text{Tr} \left(\chi_u \phi [D^2 - V(u) + C L_1^2] \phi \chi_u \gamma_u \right) \frac{du}{L_1^3} - \int \int \varrho_{\gamma_u}(x) \nabla V(u) \cdot (x - u) \phi^2(x) \chi_u^2(x) \frac{du}{L_1^3} dx \\ &\leq \int \text{Tr} \left(\chi_u^2 \phi^2 [D^2 - V(u) + C h^2 L_1^{-2} + C L_1^2] \gamma_u \right) \frac{du}{L_1^3} \\ &\quad - c_1 h^{-3} \int \int [V(u) - C(h^2 L_1^{-2} + L_1^2)]_+^{3/2} \nabla V(u) \cdot (x - u) \phi^2(x) \chi_u^2(x) \frac{du}{L_1^3} dx \\ &\leq \int \text{Tr} \left(\chi_u \phi [D^2 - V(u) + C h^2 L_1^{-2} + C L_1^2]_- \phi \chi_u \right) \frac{du}{L_1^3} + C L_1^2 h^{-3} \int \phi^2 \\ &\leq \int \text{Tr} \left(\chi_u \phi [D^2 - V(u)]_- \phi \chi_u \right) \frac{du}{L_1^3} + C(h^2 L_1^{-2} + L_1^2) h^{-3} \int \phi^2. \end{aligned} \tag{6.24}$$

In the last but one step we used (6.7) and that

$$[V(u) - C(h^2 L_1^{-2} + L_1^2)]_+^{3/2} \nabla V(u) = [V(x) - C(h^2 L_1^{-2} + L_1^2)]_+^{3/2} \nabla V(x) + O(L_1)$$

if $|x - u| \leq C L_1$. In the last step we used an estimate similar to (6.17). This proves (6.3) and completes the proof of Theorem 6.1, assuming Theorem 6.4 to be proven in the next section. \square

6.2 Removing A

In this section we estimate the effect of removing the vector potential from the operator $H(A) = T_h(A) - W$ with a constant potential $W > 0$ on a scale L . In the applications, L will be $L_1 = h^{1/2+\varepsilon_0}$. Let $H_0 = H(A=0) = D^2 - W$ and define the free projection

$$P = \mathbf{1}_{(-\infty, 0]}(H_0). \quad (6.25)$$

We also set $\Lambda_L := h^{-3}L^3$.

Theorem 6.4. *Given $0 \leq \alpha < 1$ and $0 < \varepsilon < \frac{1}{2}(1 - \alpha)$, let L be a lengthscale that satisfies*

$$h^{1-\frac{\alpha}{2}-\varepsilon}W^{-1/2} \leq L \leq Ch^{1/2}(|\log h|)^{-2}W^{-1/2}. \quad (6.26)$$

Let η be a smooth cutoff function supported on $B(L)$ with $|\partial^n \eta| \leq C_n L^{-n}$. Let $A \in H_{\text{loc}}^1(\mathbb{R}^3)$ be a vector potential. We will assume the gauge to be such that $\nabla \cdot A = 0$ on $B(5L/4)$ and

$$\int_{B(2L)} A = 0. \quad (6.27)$$

We also assume that

$$h^{-2}W^{1/2} \int_{B(2L)} |\nabla \otimes A|^2 \leq CW^{5/2}\Lambda_L. \quad (6.28)$$

Then for any $\delta > 0$ there exists $C_{\delta, \varepsilon}$, depending also on the constants in (6.26) and (6.28), such that for any density matrix $0 \leq \gamma \leq 1$ we have

$$\text{Tr } H(A)\eta\gamma\eta = \text{Tr } [T_h(A) - W]\eta\gamma\eta \geq \text{Tr } \eta[H_0]_-\eta - C_{\delta, \varepsilon}h^\alpha W^{5/2}\Lambda_L - C\delta h^{-2}W^{1/2} \int_{B(2L)} |\nabla \otimes A|^2. \quad (6.29)$$

Remark 6.5. *The gauge choice (6.27) implies that one can use the Poincaré inequality on $B(2L)$ to conclude that*

$$\int_{B(2L)} A^2 \leq CL^2 \int_{B(2L)} |\nabla \otimes A|^2. \quad (6.30)$$

Proof of Theorem 6.4. We start with localizing the vector potential which will be used later. Let ϕ' be a standard localization function on $B(5L/4)$, i.e. $\phi' \equiv 1$ on $B(5L/4)$, $\text{supp } \phi' \subset B(3L/2)$, and define

$$A' := \phi' A, \quad (6.31)$$

in particular $\nabla \cdot A' = 0$ on $B(5L/4)$. Note that this definition of A' is different from (6.19) used in the proof of Theorem 6.1 in Section 6.1; the prime notation will always indicate a

trivial cutoff outside of the appropriate domain we actually work on. In Section 6.2 we will use (6.31).

We have $\eta A = \eta A'$, so the sole purpose of this modification is to guarantee that only the local part of A will be taken into account. The Poincaré inequality (6.30) remains valid in the form

$$\int [A']^2 \leq \int_{B(2L)} A^2 \leq CL^2 \int_{B(2L)} |\nabla \otimes A|^2. \quad (6.32)$$

6.2.1 Decomposition in energy space

We introduce a dyadic decomposition around the non-magnetic Fermi surface using cutoff functions in energy space. The final result of this section is given in Lemma 6.7.

Let χ_i , $i > 0$, be smooth cutoff functions such that $\text{supp } \chi_i \subset [\frac{3}{4} \cdot 2^{i-1}, \frac{5}{4} \cdot 2^i]$, $\chi_i \leq 1$, $\chi_i(t) = 1$ for $t \in [\frac{5}{4} \cdot 2^{i-1}, \frac{3}{4} \cdot 2^i]$, $|\nabla \chi_i| \leq C \cdot 2^{-i}$ and

$$\sum_{i \geq 1} \chi_i^2(t) \equiv 1, \quad \forall t > 2.$$

Define cutoff functions on \mathbb{R}^3 by

$$f_i(u) = \chi_i\left(\frac{u^2 - W}{wW}\right) \quad \text{for } i > 0, \quad u \in \mathbb{R}^3$$

and

$$f_i(u) = \chi_{|i|}\left(-\frac{u^2 - W}{wW}\right) \quad \text{for } i < 0, \quad u \in \mathbb{R}^3,$$

with some w such that $h \leq w \leq 1$. Setting $i_0 := \lceil |\log_2 w| \rceil + 1$, where $\lceil \cdot \rceil$ denotes the integer part, we clearly have $f_i \equiv 0$ if $i < -i_0$. Define $w_i := 2^{|i|}w$, then f_i is supported in a spherical shell of volume $Cw_iW^{3/2}$ for $|i| \leq i_0$.

Clearly

$$\sum_{i > 0} f_i^2 + \sum_{i < 0} f_i^2 \leq 1$$

so we can define

$$f_0(u) = \chi_0\left(\frac{u^2 - W}{wW}\right)$$

with an appropriate cutoff function χ_0 , with $0 \leq \chi_0 \leq 1$, $|\nabla \chi_0| \leq C$, so that

$$\sum_{i \in \mathbb{Z}} f_i^2 \equiv 1,$$

i.e., $f_0(u)$ is supported in the regime where $|u^2 - W| \leq \frac{5}{4}wW$ and $f_0(u) \equiv 1$ where $|u^2 - W| \leq \frac{3}{4}wW$. Note that

$$f_i f_j \equiv 0, \quad \text{if } |i - j| \geq 2.$$

We also define $f_>$ by

$$f_>^2 := \sum_{i>i_0} f_i^2.$$

We note that the support of $f_>(t)$ lies entirely in the regime $|t| \geq 2$ and

$$|\nabla f_>| \leq C, \quad |\text{supp}(\nabla f_>)| \leq C. \quad (6.33)$$

For each i with $0 < |i| \leq i_0$ we also define enlarged cutoff functions \tilde{f}_i by

$$\tilde{f}_i(u) = \tilde{\chi}_i \left(\frac{u^2 - W}{wW} \right) \quad \text{for } i > 0$$

and

$$\tilde{f}_i(u) = \tilde{\chi}_{|i|} \left(-\frac{u^2 - W}{wW} \right) \quad \text{for } i < 0,$$

where $\tilde{\chi}_i, i > 0$, are cutoff functions such that $\text{supp } \tilde{\chi}_i \subset [\frac{1}{2} \cdot 2^{i-1}, \frac{3}{2} \cdot 2^i]$, $\chi_i \leq 1$, $\tilde{\chi}_i(t) = 1$ for $t \in [\frac{3}{4} \cdot 2^{i-1}, \frac{5}{4} \cdot 2^i]$ and $|\nabla \tilde{\chi}_i| \leq C \cdot 2^{-i}$. We also set

$$\tilde{f}_0(u) = \tilde{\chi}_0 \left(\frac{u^2 - W}{wW} \right),$$

where $\tilde{\chi}_0 \leq 1$, $\tilde{\chi}_0(t) \equiv 1$ for $|t| \leq 2$, $\text{supp } \tilde{\chi}_0 \subset [-3, 3]$ and $|\nabla \tilde{\chi}_0| \leq C$. We can similarly define $\tilde{f}_>$ by

$$\tilde{f}_>^2 := \sum_{i \geq i_0} f_i^2.$$

Note that $\tilde{\chi}_i \equiv 1$ on the support of χ_i , therefore we have

$$f_i \tilde{f}_i = f_i, \quad 0 \leq |i| \leq i_0, \quad \text{and} \quad f_> \tilde{f}_> = f_>. \quad (6.34)$$

These extended functions clearly satisfy

$$\tilde{f}_i \leq f_{i-1} + f_i + f_{i+1} \quad \text{for } |i| < i_0, \quad (6.35)$$

$$\tilde{f}_{i_0} \leq f_{i_0-1} + f_{i_0} + f_> \quad (6.36)$$

and $0 \leq \tilde{f}_i \leq 1, 0 \leq \tilde{f}_> \leq 1$.

Finally we define the momentum cutoff operators by

$$F_i := f_i(D), \quad F_> := f_>(D), \quad \tilde{F}_i := \tilde{f}_i(D), \quad \tilde{F}_> := \tilde{f}_>(D), \quad (6.37)$$

then all inequalities (6.34), (6.35) and (6.36) are clearly satisfied as operator inequalities if the functions f are replaced with the operators F .

In the first step, we neglect the positive A^2 term:

$$\mathrm{Tr} H(A)\eta\gamma\eta \geq \mathrm{Tr} \tilde{H}(A)\eta\gamma\eta$$

with

$$\tilde{H}(A) := H_0 + \sigma(D)\sigma(A) + \sigma(A)\sigma(D) = H_0 + 2DA + h\sigma(B) \quad (6.38)$$

using $\nabla \cdot A = 0$ on the support of η and $\nabla \times A = B$ in the last identity and introducing the shorter notation $\sigma(v) = \boldsymbol{\sigma} \cdot v$ for any vector v . Note that the formula (6.38) holds if the kinetic energy $T_h(A)$ is the Pauli operator, for the Schrödinger case we would have the simpler formula

$$\tilde{H}(A) := H_0 + DA + AD = H_0 + 2DA.$$

Here we adopted the convention that $DA = \sum_{j=1}^3 (-ih\nabla_j)A_j$, $AD = \sum_{j=1}^3 A_j(-ih\nabla_j)$ and $D \cdot A = \sum_{j=1}^3 -ih(\nabla_j A_j) = -ih \operatorname{div} A$, in particular, $[D, A] = D \cdot A$.

Remark 6.6. We remark that neglecting A^2 is affordable since γ is close to the projection P , defined in (6.25), and the density of the projection $\varrho_P(x)$ is bounded by $Ch^{-3}W^{3/2}$, thus

$$\begin{aligned} \mathrm{Tr} A^2\eta\gamma\eta &\approx \int A^2\eta^2\varrho_P = ch^{-3}W^{3/2} \int A^2\eta^2 \leq ch^{-3}L^2W^{3/2} \int_{B(2L)} |\nabla \otimes A|^2 \\ &= (h^{-1}L^2W)h^{-2}W^{1/2} \int_{B(2L)} |\nabla \otimes A|^2 \ll h^{-2}W^{1/2} \int_{B(2L)} |\nabla \otimes A|^2 \end{aligned}$$

by the Poincaré inequality (6.30) and $L \ll h^{1/2}W^{-1/2}$ (see (6.26)).

By the reality of the projection P , and since it acts like a scalar in spinor space, we have

$$\mathrm{Tr} [\sigma(D)\sigma(A) + \sigma(A)\sigma(D) + \sigma(B)]\eta P\eta = \mathrm{Tr} (DA + AD)\eta P\eta = 0. \quad (6.39)$$

Thus we get

$$\begin{aligned} \mathrm{Tr} H(A)\eta\gamma\eta &\geq \mathrm{Tr} \tilde{H}(A)\eta\gamma\eta - \mathrm{Tr} [\sigma(D)\sigma(A) + \sigma(A)\sigma(D)]\eta P\eta \\ &= \mathrm{Tr} F_0^2 H_0 \eta\gamma\eta + \mathrm{Tr} F_0^2 [\sigma(D)\sigma(A) + \sigma(A)\sigma(D)]\eta(\gamma - P)\eta + \mathrm{Tr} (1 - F_0^2)H_0\eta P\eta \\ &\quad + \sum_{i<0} \mathrm{Tr} F_i^2 \tilde{H}(A)\eta(\gamma - 1)\eta - \sum_{i<0} \mathrm{Tr} F_i^2 \tilde{H}(A)\eta(P - 1)\eta \\ &\quad + \sum_{i>0} \mathrm{Tr} F_i^2 \tilde{H}(A)\eta\gamma\eta - \sum_{i>0} \mathrm{Tr} F_i^2 \tilde{H}(A)\eta P\eta. \end{aligned} \quad (6.40)$$

The combination of the first and third term on the r.h.s of (6.40) gives the main term in (6.29):

$$\begin{aligned} \mathrm{Tr} F_0 H_0 F_0 \eta\gamma\eta + \mathrm{Tr} H_0 (1 - F_0^2) \eta P\eta &\geq \mathrm{Tr} [\eta F_0 H_0 F_0 \eta]_- + \mathrm{Tr} [\eta (1 - F_0^2)^{1/2} H_0 (1 - F_0^2)^{1/2} \eta]_- \\ &\geq \mathrm{Tr} \eta \left([F_0 H_0 F_0]_- + [(1 - F_0^2)^{1/2} H_0 (1 - F_0^2)^{1/2}]_- \right) \eta \\ &= \mathrm{Tr} \eta [H_0]_- \eta. \end{aligned} \quad (6.41)$$

Notice that the sum on the RHS of (6.40) is real though each individual term might not be. To symmetrize some of the terms we take the real part and we have proved

Lemma 6.7. *With the notations introduced above, we have*

$$\begin{aligned} \text{Tr } H(A)\eta\gamma\eta &\geq \text{Tr } \eta[H_0]_-\eta + \Re \text{Tr } F_0^2 [\sigma(D)\sigma(A) + \sigma(A)\sigma(D)]\eta(\gamma - P)\eta \\ &\quad + \sum_{i<0} \Re \text{Tr } F_i^2 \tilde{H}(A)\eta(\gamma - 1)\eta - \sum_{i<0} \Re \text{Tr } F_i^2 \tilde{H}(A)\eta(P - 1)\eta \\ &\quad + \sum_{i>0} \Re \text{Tr } F_i^2 \tilde{H}(A)\eta\gamma\eta - \sum_{i>0} \Re \text{Tr } F_i^2 \tilde{H}(A)\eta P\eta. \quad \square \end{aligned} \quad (6.42)$$

The main term is the first on the r.h.s of (6.42). In the next subsections we estimate the other terms and we show that they can be included in the negative error terms in (6.29).

6.2.2 Estimate of the $\sigma(D)\sigma(A) + \sigma(A)\sigma(D)$ term in (6.42)

Lemma 6.8. *For any $\delta > 0$ we have*

$$\begin{aligned} &\left| \text{Tr } F_0^2 [\sigma(D)\sigma(A) + \sigma(A)\sigma(D)]\eta(\gamma - P)\eta \right| \\ &\leq C\delta^{-1} [h + wLW^{1/2} + h^{-1}w^2L^2W] W^{5/2} \Lambda_L + \delta h^{-2} W^{1/2} \int_{B(2L)} |\nabla \otimes A|^2. \end{aligned} \quad (6.43)$$

Proof. Using $\nabla \cdot A = 0$ on $B(5L/4)$ and $\eta A = \eta A'$ (recall the definition of A' from (6.31)) and the locality of the operator D , we have

$$F_0^2 [\sigma(D)\sigma(A) + \sigma(A)\sigma(D)]\eta(\gamma - P)\eta = 2F_0^2 D A' \eta(\gamma - P)\eta + h F_0^2 \sigma(B') \eta(\gamma - P)\eta \quad (6.44)$$

with $B' = \nabla \times A'$. Note that

$$\int [B']^2 \leq CL^{-2} \int_{B(2L)} A^2 + \int_{\mathbb{R}^3} [\phi']^2 |\nabla \times A|^2 \leq C \int_{B(2L)} |\nabla \otimes A|^2 \quad (6.45)$$

using (6.27) and the Poincaré inequality.

We will estimate $|\text{Tr } F_0^2 D A' \eta\gamma\eta|$ and $|h \text{Tr } F_0^2 \sigma(B') \eta\gamma\eta|$ for any density matrix $0 \leq \gamma \leq 1$, and then the same estimate can be applied to γ replaced with P as well. We start with the second (magnetic) term in (6.44), and in fact we prove the following stronger estimate that will be used later

$$\begin{aligned} \sum_{|i| \leq i_0} h |\text{Tr } F_i^2 \sigma(B') \eta\gamma\eta| &\leq \sum_{|i| \leq i_0} h \left(\text{Tr } F_i^2 [B']^2 \right)^{1/2} \left(\text{Tr } F_i^2 \eta\gamma\eta \right)^{1/2} \\ &\leq \sum_{|i| \leq i_0} C h^{-2} w_i W^{3/2} \left(\int [B']^2 \right)^{1/2} \left(\int \eta^2 \right)^{1/2} \\ &\leq \delta h^{-2} W^{1/2} \int_{B(2L)} |\nabla \otimes A|^2 + C \delta^{-1} h W^{5/2} \Lambda_L. \end{aligned} \quad (6.46)$$

Here we used (6.45) and that the diagonal element of F_i , $|i| \leq i_0$, is bounded by

$$\sup_x F_i(x, x) \leq \int_{\mathbb{R}^3} f_i(hp) dp \leq Ch^{-3}w_i W^{3/2} \quad (6.47)$$

since the support of f_i is a spherical shell of width $Cw_i W^{1/2}$ and radius of order $W^{1/2}$, where we recall $w_i = 2^{|i|}w$. In particular, (6.46) shows that the magnetic term in (6.44) can be estimated as required in Lemma 6.8.

For the first term in (6.44), with a general density matrix γ , we insert \tilde{F}_0 and $\tilde{G}_0 := 1 - \tilde{F}_0$ to get

$$|\mathrm{Tr} F_0^2 DA' \eta \gamma \eta| \leq |\mathrm{Tr} F_0^2 DA' \tilde{F}_0 \eta \gamma \eta \tilde{F}_0| + |\mathrm{Tr} F_0^2 A' \tilde{G}_0 \eta \gamma \eta \tilde{F}_0 D|, \quad (6.48)$$

where we used (6.34) and the cyclicity of the trace. We will estimate these two terms separately.

The first term in (6.48) is estimated as

$$\begin{aligned} |\mathrm{Tr} F_0^2 DA' \tilde{F}_0 \eta \gamma \eta \tilde{F}_0| &\leq \left(\mathrm{Tr} [A']^2 \tilde{F}_0 \eta \gamma \eta \tilde{F}_0 \right)^{1/2} \left(\mathrm{Tr} F_0^4 D^2 \tilde{F}_0 \eta \gamma \eta \tilde{F}_0 \right)^{1/2} \\ &\leq C \left(\mathrm{Tr} [A']^2 \tilde{F}_0^2 \right)^{1/2} \left(W \mathrm{Tr} F_0^4 \eta^2 \right)^{1/2} \\ &\leq Ch^{-3}wW^2 \left(\int [A']^2 \right)^{1/2} \left(\int \eta^2 \right)^{1/2} \\ &\leq \delta^{-1}h^{-1}w^2L^2W^{7/2}\Lambda_L + \delta h^{-2}W^{1/2} \int_{B(2L)} |\nabla \otimes A|^2. \end{aligned} \quad (6.49)$$

Here we first used that D^2 is bounded by CW when multiplied by F_0 . Then, similarly to (6.47), we estimated the diagonal element of F_0 and \tilde{F}_0 as

$$\sup_x F_0(x, x) \leq \sup_x \tilde{F}_0(x, x) \leq Ch^{-3}wW^{3/2}, \quad (6.50)$$

and finally we used (6.32).

The second term in (6.48) is estimated as

$$|\mathrm{Tr} F_0^2 A' \tilde{G}_0 \eta \gamma \eta \tilde{F}_0 D| \leq \left(\mathrm{Tr} F_0^2 A' \tilde{G}_0^2 A' F_0^2 \right)^{1/2} \left(\mathrm{Tr} D^2 \tilde{F}_0^2 (\eta \gamma \eta)^2 \right)^{1/2}. \quad (6.51)$$

For the second factor we can use the previous bound

$$\mathrm{Tr} D^2 \tilde{F}_0^2 (\eta \gamma \eta)^2 \leq CW \mathrm{Tr} \tilde{F}_0^2 \eta^2 \leq Ch^{-3}wW^{5/2}L^3 = CwW^{5/2}\Lambda_L. \quad (6.52)$$

To estimate the first factor, we will need the following lemma, whose proof is postponed:

Lemma 6.9. *Let f and g be positive real functions on \mathbb{R}^3 such that $fg = 0$. Then for any real function $a \in H^1(\mathbb{R}^3)$ we have*

$$\mathrm{Tr}_{L^2(\mathbb{R}^3)} [f(D)a(x)g(D)a(x)f(D)] \leq h^{-2} \|f\|_\infty \|g\|_\infty \|\nabla f\|_1 \|a\|_2 \|\nabla \otimes a\|_2. \quad (6.53)$$

Using that $F_0 = f_0(D)$ with a function f_0 satisfying $|\nabla f_0| \leq Cw^{-1}W^{-1/2}$, $|\text{supp } f_0| \leq CwW^{3/2}$, thus $\|\nabla f_0\|_1 \leq CW$, we obtain

$$\text{Tr } F_0^2 A' \tilde{G}_0^2 A' F_0^2 \leq Ch^{-2}W \|A'\|_2 \|\nabla \otimes A'\|_2 \leq Ch^{-2}LW \int_{B(2L)} |\nabla \otimes A|^2. \quad (6.54)$$

Here we used (6.32) and the second inequality in (6.45).

Combining these estimates and separating the two factors in (6.51) by a Schwarz inequality we obtain the following bound

$$|\text{Tr } F_0^2 A' \tilde{G}_0 \eta \gamma \eta \tilde{F}_0 D| \leq C\delta^{-1}wLW^3\Lambda_L + \delta h^{-2}W^{1/2} \int_{B(2L)} |\nabla \otimes A|^2. \quad (6.55)$$

This completes the proof of Lemma 6.8. \square

Proof of Lemma 6.9. By passing to Fourier space we get

$$\text{Tr }_{L^2(\mathbb{R}^3)} [f(D)a(x)g(D)a(x)f(D)] = \iint_{\mathbb{R}^3 \times \mathbb{R}^3} f(hp)\hat{a}(p-q)g(hq)\hat{a}(q-p)f(hp) \, dpdq. \quad (6.56)$$

We now use that $fg = 0$ to rewrite the above integral as

$$\begin{aligned} &= \iint [f(hp) - f(hq)] |\hat{a}(p-q)|^2 g(hq) f(hp) \, dpdq \\ &\leq \|f\|_\infty \|g\|_\infty \iint \int_0^1 |h(q-p) \cdot \nabla f(hp + th(q-p))| \, dt |\hat{a}(p-q)|^2 \, dpdq \\ &= h^{-2} \|f\|_\infty \|g\|_\infty \int_{\mathbb{R}^3} |\nabla f(v)| \, dv \int_{\mathbb{R}^3} |z| |\hat{a}(z)|^2 \, dz. \end{aligned} \quad (6.57)$$

The result now follows upon passing back in x -space in the integral over \hat{a} . \square

6.2.3 Error terms in (6.42) for $i > i_0$

We now deal with the two sums in the last line of (6.42) in the regime where $i > i_0$.

Lemma 6.10. *Under the conditions $LW^{1/2} \ll h^{1/2}$ and assuming (6.28), we have for any fixed $\delta > 0$*

$$\Re \sum_{i > i_0} \text{Tr } F_i^2 \tilde{H}(A) \eta \gamma \eta \geq \frac{1}{2} \text{Tr } [D^2 F_{>}^2 \eta \gamma \eta] - C\delta h^{-2}W^{1/2} \int_{B(2L)} |\nabla \otimes A|^2 - \delta \text{Tr } [D^2 \tilde{F}_{>}^2 \eta \gamma \eta] \quad (6.58)$$

if $h \leq h_\delta$. Moreover, for any $N \geq 1$ and $h \leq h_\delta$, we also have

$$\left| \sum_{i > i_0} \text{Tr } F_i^2 \tilde{H}(A) \eta P \eta \right| \leq C\delta h^{-2}W^{1/2} \int_{B(2L)} |\nabla \otimes A|^2 + C_N W^{5/2} \left(\frac{h}{LW^{1/2}} \right)^N. \quad (6.59)$$

Proof. Using the first formula in (6.38), we write

$$\begin{aligned} \Re \sum_{i>i_0} \text{Tr } F_i^2 \tilde{H}(A) \eta \gamma \eta &= \Re \text{Tr } F_{>}^2 [H_0 + \sigma(D)\sigma(A) + \sigma(A)\sigma(D)] \eta \gamma \eta \\ &\geq \frac{1}{2} \text{Tr } [D^2 F_{>}^2 \eta \gamma \eta] - |\text{Tr } F_{>}^2 \sigma(D)\sigma(A') \eta \gamma \eta| - |\text{Tr } F_{>}^2 \sigma(A')\sigma(D) \eta \gamma \eta|. \end{aligned} \quad (6.60)$$

Inserting $\tilde{G}_{>} := 1 - \tilde{F}_{>}$ into the second term, and using (6.34), we have

$$|\text{Tr } F_{>}^2 \sigma(D)\sigma(A') \eta \gamma \eta| \leq |\text{Tr } F_{>}^2 \sigma(D)\sigma(A') \tilde{F}_{>} \eta \gamma \eta \tilde{F}_{>}| + |\text{Tr } F_{>}^2 \sigma(A') \tilde{G}_{>} \eta \gamma \eta \tilde{F}_{>} \sigma(D)|. \quad (6.61)$$

For the first term in (6.61), with the notation $\tilde{\omega}_{>} := \tilde{F}_{>} \eta \gamma \eta \tilde{F}_{>}$, we use

$$|\text{Tr } F_{>}^2 \sigma(D)\sigma(A') \tilde{F}_{>} \eta \gamma \eta \tilde{F}_{>}| \leq \left(\text{Tr } [A']^2 \tilde{\omega}_{>} \right)^{1/2} \left(\text{Tr } D^2 \tilde{\omega}_{>} \right)^{1/2}. \quad (6.62)$$

Applying Hölder, Sobolev and Lieb-Thirring inequalities and the bounds (6.32), (6.45), we have

$$\begin{aligned} \text{Tr } [A']^2 \tilde{\omega}_{>} &\leq \left(\int [A']^5 \right)^{2/5} \left(\int \tilde{\varrho}_{>}^{5/3} \right)^{3/5} \\ &\leq C \left(\int [A']^2 \right)^{1/10} \left(\int [A']^6 \right)^{3/10} \left(h^{-2} \text{Tr } D^2 \tilde{\omega}_{>} \right)^{3/5} \\ &\leq CL^{1/5} \left(\int_{B(2L)} |\nabla \otimes A|^2 \right) \left(h^{-2} \text{Tr } D^2 \tilde{\omega}_{>} \right)^{3/5}, \end{aligned} \quad (6.63)$$

where $\tilde{\varrho}_{>}(x) := \tilde{\omega}_{>}(x, x)$ denotes the density of $\tilde{\omega}_{>}$. Thus (6.62) can be estimated as

$$\begin{aligned} |\text{Tr } F_{>}^2 \sigma(D)\sigma(A') \tilde{F}_{>} \eta \gamma \eta \tilde{F}_{>}| &\leq CL^{1/10} h^{-3/5} \left(\int_{B(2L)} |\nabla \otimes A|^2 \right)^{1/2} \left(\text{Tr } D^2 \tilde{\omega}_{>} \right)^{4/5} \\ &\leq C_\delta L^{1/2} h^{-3} \left(\int_{B(2L)} |\nabla \otimes A|^2 \right)^{5/2} + \delta \text{Tr } D^2 \tilde{\omega}_{>} \\ &\leq C_\delta (h^{-1/2} L)^5 h^{-2} W^3 \int_{B(2L)} |\nabla \otimes A|^2 + \delta \text{Tr } D^2 \tilde{\omega}_{>}, \end{aligned} \quad (6.64)$$

where we used (6.28) in the last step. Considering that $LW^{1/2} \ll h^{1/2}$, we obtain that the first term in (6.61) is bounded by the two negative error terms in (6.58).

For the second term in (6.61), after a Schwarz inequality, we use Lemma 6.9 similarly to (6.54):

$$\begin{aligned} |\text{Tr } F_{>}^2 \sigma(A') \tilde{G}_{>} \eta \gamma \eta \tilde{F}_{>} \sigma(D)| &\leq \left(\text{Tr } F_{>}^2 A' \tilde{G}_{>}^2 A' F_{>}^2 \right)^{1/2} \left(\text{Tr } D^2 \tilde{F}_{>}^2 (\eta \gamma \eta)^2 \right)^{1/2} \\ &\leq C \left(L h^{-2} W \int_{B(2L)} |\nabla \otimes A|^2 \right)^{1/2} \left(\text{Tr } D^2 \tilde{F}_{>}^2 \eta \gamma \eta \right)^{1/2} \\ &\leq C \delta h^{-3/2} W^{1/2} \int_{B(2L)} |\nabla \otimes A|^2 + \delta \text{Tr } D^2 \tilde{F}_{>}^2 \eta \gamma \eta \end{aligned} \quad (6.65)$$

for $h \leq h_\delta$, using $LW^{1/2} \ll h^{1/2}$ and estimating $\|\nabla f_\gamma\|_1 \leq CW$. Therefore the second term in (6.61) is also bounded by the two negative error terms in (6.58).

We now estimate the third term in (6.60):

$$\begin{aligned}
|\text{Tr } F_\gamma^2 \sigma(A') \sigma(D) \eta \gamma \eta| &\leq |\text{Tr } F_\gamma^2 \sigma(A') \tilde{F}_\gamma \sigma(D) \eta \gamma \eta| + |\text{Tr } F_\gamma^2 \sigma(A') \tilde{G}_\gamma \sigma(D) \eta \gamma \eta| \\
&\leq \left(\text{Tr } F_\gamma^2 \sigma(A')^2 F_\gamma^2 \tilde{\omega}_\gamma \right)^{1/2} \left(\text{Tr } D^2 \tilde{\omega}_\gamma \right)^{1/2} \\
&\quad + \left(\text{Tr } F_\gamma^2 \sigma(A') \tilde{G}_\gamma \sigma(A') F_\gamma^2 \right)^{1/2} \left(\text{Tr } \tilde{F}_\gamma \eta \gamma \eta \sigma(D) \tilde{G}_\gamma \sigma(D) \eta \gamma \eta \tilde{F}_\gamma \right)^{1/2} \\
&\leq C \left(\text{Tr } [A']^2 F_\gamma^2 \tilde{\omega}_\gamma F_\gamma^2 \right)^{1/2} \left(\text{Tr } D^2 \tilde{\omega}_\gamma \right)^{1/2} \\
&\quad + C \left(\text{Tr } F_\gamma^2 A' \tilde{G}_\gamma A' F_\gamma^2 \right)^{1/2} \left(\text{Tr } D^2 \tilde{\omega}_\gamma \right)^{1/2}.
\end{aligned} \tag{6.66}$$

Here we used that $F_\gamma^2 = F_\gamma^2 \tilde{F}_\gamma^2$ and that $\sigma(D) \tilde{G}_\gamma \sigma(D) = D^2 \tilde{G}_\gamma \leq D^2$. The second term in the r.h.s of (6.66) is estimated exactly as (6.65). For the first term we essentially repeat the estimate (6.63):

$$\text{Tr } [A']^2 F_\gamma^2 \tilde{\omega}_\gamma F_\gamma^2 \leq CL^{1/5} \left(\int_{B(2L)} |\nabla \otimes A|^2 \right) \left(h^{-2} \text{Tr } D^2 \tilde{\omega}_\gamma \right)^{3/5}$$

after estimating $\text{Tr } D^2 F_\gamma^2 \tilde{\omega}_\gamma F_\gamma^2 \leq \text{Tr } D^2 \tilde{\omega}_\gamma$. This completes the proof of (6.58).

For the proof of (6.59), we write

$$|\text{Tr } F_\gamma^2 \tilde{H}(A) \eta P \eta| \leq |\text{Tr } F_\gamma^2 H_0 \eta P \eta| + 2 |\text{Tr } F_\gamma^2 [\sigma(D) \sigma(A') + \sigma(A') \sigma(D)] \eta P \eta|.$$

Notice that in the estimate of the $\sigma(D) \sigma(A')$ and $\sigma(A') \sigma(D)$ terms on the r.h.s of (6.60) explained above is valid for any density matrix γ , in particular also for $\gamma = P$, thus

$$|\text{Tr } F_\gamma^2 \tilde{H}(A) \eta P \eta| \leq (1 + \delta) |\text{Tr } \tilde{F}_\gamma^2 H_0 \eta P \eta| + C \delta h^{-2} W^{1/2} \int_{B(2L)} |\nabla \otimes A|^2. \tag{6.67}$$

On the support of \tilde{F}_γ we have $|H_0| \leq 2D^2$, thus $\text{Tr } \tilde{F}_\gamma^2 H_0 \eta P \eta \leq 2 \text{Tr } D \tilde{F}_\gamma \eta P \eta \tilde{F}_\gamma D$. To estimate $\text{Tr } D \tilde{F}_\gamma \eta P \eta \tilde{F}_\gamma D$, we use (6.72) from Lemma 6.11 below. We set $\ell := hW^{-1/2}$, $f(p) := \tilde{f}_\gamma(W^{1/2}p)p$ and $g(p) := \mathbf{1}(|p| \leq 1)$, so that $\tilde{F}_\gamma(D)D = W^{1/2}f(-i\ell\nabla)$ and $P = g(-i\ell\nabla)$

$$\text{Tr } D \tilde{F}_\gamma \eta P \eta \tilde{F}_\gamma D = \|D \tilde{F}_\gamma \eta P\|_{HS}^2 \leq C_N W^{5/2} \left(\frac{h}{LW^{1/2}} \right)^N \tag{6.68}$$

using that the supports of f and g are separated by a distance d of order one. The condition $\ell \leq Ld$ is guaranteed by (6.26). Upon combining this with (6.67) we have completed the proof of Lemma 6.10. \square

Lemma 6.11. *Let f and g be real functions so that their supports are separated by d , i.e.*

$$\text{dist}(\text{supp}(f), \text{supp}(g)) \geq d. \quad (6.69)$$

Let $\eta(x) := \eta_0(x/L)$ with $L > 0$, where η_0 is a smooth function with compact support. Then for any $N > 0$ and $\ell \leq Ld$ we have the following bounds

$$\|f(-i\ell\nabla)\eta g(-i\ell\nabla)\|_{HS} \leq C_N \left(\frac{\ell}{dL}\right)^N \left(\frac{L}{\ell}\right)^3 \|f\|_2 \|g\|_2 \quad (6.70)$$

and

$$\|f(-i\ell\nabla)\eta g(-i\ell\nabla)\|_{HS} \leq C_N \left(\frac{\ell}{dL}\right)^N \left(\frac{L}{\ell}\right)^{3/2} \|f\|_2 \|g\|_\infty, \quad (6.71)$$

$$\|f(-i\ell\nabla)\eta g(-i\ell\nabla)\|_{HS} \leq C_N \left(\frac{\ell}{dL}\right)^N \left(\frac{L}{\ell}\right)^3 \left\| \frac{f(p)}{1+p^2} \right\|_\infty \|g(p)(1+p^2)^3\|_\infty \quad (6.72)$$

where C_N depends only on η_0 and N .

Proof. Since $\eta_0 \in C_0^\infty$, we have

$$|\widehat{\eta}_0(p)| \leq C_N (1+p^2)^{-N/2}$$

for any $N \geq 0$. We compute in Fourier space, using that $\widehat{\eta}(p) = L^3 \widehat{\eta}_0(pL)$ (with an appropriate convention about the 2π), and (6.69), we get

$$\begin{aligned} \|f(-i\ell\nabla)\eta g(-i\ell\nabla)\|_{HS}^2 &= \iint dp dq |f(\ell p)|^2 |\widehat{\eta}(p-q)|^2 |g(\ell q)|^2 \\ &= (L/\ell)^6 \iint dp dq |f(p)|^2 |\widehat{\eta}_0((p-q)L/\ell)|^2 |g(q)|^2 \\ &\leq C_N (L/\ell)^6 \iint dp dq \frac{|f(p)|^2 |g(q)|^2}{[1+(p-q)^2(L/\ell)^2]^N} \\ &\leq C_N (\ell/Ld)^{2N} \left(\frac{L}{\ell}\right)^6 \|f\|_2^2 \|g\|_2^2 \end{aligned} \quad (6.73)$$

which proves (6.70). For the proof of (6.71), we extract a decay of order $(\ell/Ld)^{2N-4}$, estimate $|g(q)| \leq \|g\|_\infty$ and then integrate out q . The proof of (6.72) is similar:

$$\begin{aligned} &\|f(D)\eta g(D)\|_{HS}^2 \\ &\leq C_N \left\| \frac{f(p)}{1+p^2} \right\|_\infty^2 \|g(q)(1+q^2)^3\|_\infty^2 \left(\frac{\ell}{Ld}\right)^{2N-6} \left(\frac{L}{\ell}\right)^6 \iint dp dq \frac{(1+p^2)}{(1+q^2)^3 [1+(p-q)^2]^3} \end{aligned} \quad (6.74)$$

and the last integral is finite. This completes the proof of Lemma 6.11. \square

6.2.4 Error terms in (6.42) for $|i| \leq i_0$

In Lemma 6.10 we have estimated the terms $i > i_0$ in the last two summations in (6.42). Note that the terms with $i < -i_0$ in the second line of (6.42) identically vanish. It now remains to estimate the last four sums in (6.42) for $0 < |i| \leq i_0$.

Lemma 6.12. *Define $w_i := 2^{|i|}w$ and assume (6.26) and $LW^{1/2} \ll w$. Then for any $\delta > 0$ and $h \leq h_\delta$ we have*

$$\begin{aligned} & \sum_{0 < i \leq i_0} \Re \text{Tr } F_i^2 \tilde{H}(A) \eta \gamma \eta + \sum_{-i_0 \leq i < 0} \Re \text{Tr } F_i^2 \tilde{H}(A) \eta (\gamma - 1) \eta \\ & \geq \sum_{0 < i \leq i_0} \frac{w_i}{40} \text{Tr } [D^2 F_i^2 \eta \gamma \eta] + \sum_{-i_0 \leq i < 0} \frac{w_i}{40} \text{Tr } [D^2 F_i^2 \eta (1 - \gamma) \eta] \\ & \quad - C\delta h^{-2} W^{1/2} \int_{B(2L)} |\nabla \otimes A|^2 \end{aligned} \quad (6.75)$$

and

$$\begin{aligned} & \sum_{0 < i \leq i_0} \left| \text{Tr } F_i^2 \tilde{H}(A) \eta P \eta \right| + \sum_{-i_0 \leq i < 0} \left| \text{Tr } F_i^2 \tilde{H}(A) \eta (P - 1) \eta \right| \\ & \leq C\delta h^{-2} W^{1/2} \int_{B(2L)} |\nabla \otimes A|^2 + C_N W^{5/2} \left(\frac{h}{w L W^{1/2}} \right)^N. \end{aligned} \quad (6.76)$$

Proof of Lemma 6.12. We will present the proof for the summations over $0 < i \leq i_0$, the estimate of the negative i 's are identical. We start with the first term in (6.75). Since $w_i = 2^{|i|}w$, then $w_i \leq 2$ for $|i| \leq i_0$. Since on the support of F_i , $i > 0$, it holds that $\frac{3}{8}w_i W \leq D^2 - W \leq \frac{5}{4}w_i W$, we obtain

$$H_0 F_i^2 \geq \frac{3}{8} w_i W F_i^2 \geq \frac{3}{8} \frac{w_i D^2 F_i^2}{\frac{5}{4} w_i + 1} \geq \frac{w_i}{20} (D^2 + W) F_i^2, \quad 0 < i \leq i_0.$$

The analogous estimate for negative i will be

$$H_0 F_i^2 \leq -\frac{3}{8} w_i W F_i^2 \leq -\frac{w_i}{20} (D^2 + W) F_i^2, \quad 0 > i \geq -i_0.$$

The additional W is necessary only for $i < 0$, when $\text{Tr } F_i \eta \gamma \eta F_i$ may not be comparable with $\text{Tr } D^2 F_i \eta \gamma \eta F_i$, but it is always comparable with $\text{Tr } (D^2 + W) F_i \eta \gamma \eta F_i$.

Using the second identity in (6.38), we have for $0 < i \leq i_0$,

$$\begin{aligned} \Re \text{Tr } F_i^2 \tilde{H}(A) \eta \gamma \eta &= \text{Tr } F_i^2 H_0 \eta \gamma \eta + 2 \Re \text{Tr } F_i^2 D A' \eta \gamma \eta + h \Re \text{Tr } F_i^2 \sigma(B) \eta \gamma \eta \\ &\geq \frac{w_i}{20} \text{Tr } (D^2 + W) F_i \eta \gamma \eta F_i - 2 |\text{Tr } F_i^2 D A' \eta \gamma \eta| - h |\text{Tr } F_i^2 \sigma(B') \eta \gamma \eta|. \end{aligned} \quad (6.77)$$

The last term was already treated in (6.46) even after summation over i .

To control the DA' error term, we proceed as before in (6.48) and (6.61) by inserting $\tilde{G}_i := 1 - \tilde{F}_i$:

$$|\mathrm{Tr} F_i^2 DA' \eta \gamma \eta| \leq |\mathrm{Tr} F_i^2 DA' \tilde{F}_i \eta \gamma \eta \tilde{F}_i| + |\mathrm{Tr} F_i^2 A' \tilde{G}_i \eta \gamma \eta \tilde{F}_i D|. \quad (6.78)$$

The first term is estimated similarly to (6.49):

$$\begin{aligned} |\mathrm{Tr} F_i^2 DA' \tilde{F}_i \eta \gamma \eta \tilde{F}_i| &\leq \left(\mathrm{Tr} [A']^2 \tilde{F}_i \eta \gamma \eta \tilde{F}_i \right)^{1/2} \left(\mathrm{Tr} F_i^4 D^2 \tilde{F}_i \eta \gamma \eta \tilde{F}_i \right)^{1/2} \\ &\leq C \left(\mathrm{Tr} [A']^2 \tilde{F}_i^2 \right)^{1/2} \left(\mathrm{Tr} D^2 F_i \eta \gamma \eta F_i \right)^{1/2} \\ &\leq C \left(h^{-3} w_i W^{3/2} \int [A']^2 \right)^{1/2} \left(\mathrm{Tr} D^2 F_i \eta \gamma \eta F_i \right)^{1/2} \\ &\leq \delta w_i \mathrm{Tr} D^2 F_i \eta \gamma \eta F_i + C \delta^{-1} (h^{-1} L^2 W) h^{-2} W^{1/2} \int_{B(2L)} |\nabla \otimes A|^2. \end{aligned} \quad (6.79)$$

Here we used $F_i \tilde{F}_i = F_i$ to remove the tildes from the terms with D^2 . We also used (6.32) and the estimate

$$\sup_x F_i(x, x) \leq \sup_x \tilde{F}_i(x, x) \leq C h^{-3} w_i W^{3/2}. \quad (6.80)$$

The second term in (6.78) is estimated similarly to (6.65) by using Lemma 6.9 and the fact that $\|\nabla f_i\|_1 \leq CW$.

$$\begin{aligned} |\mathrm{Tr} F_i^2 A' \tilde{G}_i \eta \gamma \eta \tilde{F}_i D| &\leq \left(\mathrm{Tr} F_i^2 A' \tilde{G}_i^2 A' F_i^2 \right)^{1/2} \left(\mathrm{Tr} D^2 F_i^2 \eta \gamma \eta \right)^{1/2} \\ &\leq C \left(L h^{-2} W \int_{B(2L)} |\nabla \otimes A|^2 \right)^{1/2} \left(\mathrm{Tr} D^2 F_i \eta \gamma \eta F_i \right)^{1/2} \\ &\leq \delta w_i \mathrm{Tr} D^2 F_i \eta \gamma \eta F_i + C \delta^{-1} \frac{L W^{1/2}}{w_i} h^{-2} W^{1/2} \int_{B(2L)} |\nabla \otimes A|^2. \end{aligned} \quad (6.81)$$

Summing up (6.79) and (6.81) for $i \leq i_0 \leq C|\log h|$ and using that $LW^{1/2} \ll h^{1/2}|\log h|^{-1}$ and $LW^{1/2} \ll w$, we obtain

$$\sum_{0 < i \leq i_0} |\mathrm{Tr} F_i^2 DA' \eta \gamma \eta| \leq \delta \sum_{0 < i \leq i_0} w_i \mathrm{Tr} D^2 F_i \eta \gamma \eta F_i + \delta h^{-2} W^{1/2} \int_{B(2L)} |\nabla \otimes A|^2 \quad (6.82)$$

if $h \leq h_\delta$. Combining (6.82) with the positive terms from (6.77) and choosing δ sufficiently small, we obtain

$$\Re \sum_{0 < i \leq i_0} \mathrm{Tr} F_i^2 \tilde{H}(A) \eta \gamma \eta \geq \sum_{0 < i \leq i_0} \frac{w_i}{40} \mathrm{Tr} (D^2 + W) F_i \eta \gamma \eta F_i - \delta h^{-2} W^{1/2} \int_{B(2L)} |\nabla \otimes A|^2. \quad (6.83)$$

This completes the proof of (6.75). The proof of (6.76) is analogous by using that the momentum supports of F_i and P are separated, so one can apply (6.72) similarly to (6.68) to obtain

$$\left| \text{Tr } F_i^2 H_0 \eta P \eta \right| \leq \text{Tr } D F_i \eta P \eta F_i D = \|D F_i \eta P\|_{HS}^2 \leq C_N W^{5/2} \left(\frac{h}{w L W^{1/2}} \right)^N. \quad (6.84)$$

The details will be left to the reader. This completes the proof of Lemma 6.12. \square .

Inserting the estimates from Lemma 6.8, Lemma 6.10 and Lemma 6.12 into (6.42), we have proved the following

Proposition 6.13. *Under the conditions of Theorem 6.4 and assuming $LW^{1/2} \ll w$, for any $\delta > 0$ and $h \leq h_\delta$ we have*

$$\begin{aligned} \text{Tr } H(A) \eta \gamma \eta &\geq \text{Tr } \eta [H_0]_- \eta - C \delta^{-1} \left[h + w^2 \right] W^{5/2} \Lambda_L - C_N W^{5/2} \left(\frac{h}{w L W^{1/2}} \right)^N \\ &\quad + \frac{1}{100} \text{Tr } [D^2 F_{>}^2 \eta \gamma \eta] + \sum_{0 < i \leq i_0} \frac{2^i w}{100} \text{Tr } [D^2 F_i^2 \eta \gamma \eta] + \sum_{-i_0 \leq i < 0} \frac{2^{|i|} w}{100} \text{Tr } [D^2 F_i^2 \eta (1 - \gamma) \eta] \\ &\quad - C \delta h^{-2} W^{1/2} \int_{B(2L)} |\nabla \otimes A|^2. \end{aligned} \quad (6.85)$$

Finally, given $0 \leq \alpha < 1$ and $\varepsilon > 0$ as in Theorem 6.4, we choose $w = h^{\alpha/2}$ and an integer $N \geq 3\varepsilon^{-1}$, then Proposition 6.13 implies Theorem 6.4. \square

As we already mentioned, Theorem 6.4 implies Theorem 6.1.

Upon combining Proposition 6.13 with the upper bound we get bounds on the kinetic energy terms in (6.85). These bounds will be used to control the substitution of A_0 by A_r in Section 6.3.

For each fixed $u \in B(\frac{5}{4}L_0)$, we will use Theorem 6.4 with the constant potential W replaced with V_u defined in (6.11). We know that $c_0/2 \leq V_u \leq C$, so factors $W = V_u$ can be replaced by constants in the estimates. To indicate the u -dependence, we define $H^u := D^2 - V_u$. Recall that the operators F_i and $F_{>}$ defined in Section 6.2.1 depend on W . We will denote them by F_i^u and $F_{>}^u$ in case of $W = V_u$.

Theorem 6.14. *Recall that $L_0 = h^{1/2-\varepsilon_0}$ and $\alpha = 1 - 3\varepsilon_0$ with ε_0 sufficiently small. Choose $L_1 = h^{1/2+\varepsilon_0}$. If*

$$\mathcal{E}(A) \leq \mathcal{E}(0) + C' h^{1-3\varepsilon_0} \Lambda_{L_0}, \quad (6.86)$$

then,

$$\int \mathcal{T}_u \frac{du}{L_1^3} \leq C h^{1-3\varepsilon_0} \Lambda_{L_0}, \quad (6.87)$$

where \mathcal{T}_u is given by

$$\begin{aligned} \mathcal{T}_u := \frac{1}{100} \Big\{ & \text{Tr} [D^2[F_{>}^u]^2 \eta_u \gamma_u \eta_u] + \sum_{0 < i \leq i_0} 2^i w \text{Tr} [D^2[F_i^u]^2 \eta_u \gamma_u \eta_u] \\ & + \sum_{-i_0 \leq i < 0} 2^{|i|} w \text{Tr} [D^2[F_i^u]^2 \eta_u (1 - \gamma_u) \eta_u] \Big\}, \end{aligned} \quad (6.88)$$

where

$$\gamma_u := \mathbf{1}_{(-\infty, 0]} (\chi_u \phi [T_h(A - c_u) - V_u] \phi \chi_u). \quad (6.89)$$

with c_u defined in (6.9) and we set $\eta_u := \chi_u \phi$.

Proof. By (6.10)

$$\text{Tr} [\phi [T_h(A) - V] \phi]_- \geq \int \text{Tr} [\chi_u \phi [T_h(A - c_u) - V_u] \phi \chi_u]_- \frac{du}{L_1^3}, \quad (6.90)$$

with V_u from (6.11). Since $V(0) = c_0$ by (5.9) and using $L_0 \ll 1$ and the bound on ∇V , we can assume that $V \geq c_0/2$ on $B(\frac{5}{4}L_0)$. Also, using (6.86) we get as in the proof of Corollary 6.3 that

$$\frac{1}{2\kappa h^2} \int_{B(2L_0)} |\nabla \otimes A|^2 \leq C h^{1-3\varepsilon_0} \Lambda_{L_0}.$$

Therefore, (using the smallness of ε_0) the condition (6.14) is satisfied for all u in the domain of integration. Note that this is exactly the condition (6.28) in Theorem 6.4 with $W = V_u$, with $L = L_1$ and shifting the center of the ball $B(2L)$ to u . The condition (6.27) is satisfied since we consider the vector potential $A - c_u$. Finally, the condition (6.26) is satisfied by (6.13). We can thus apply Proposition 6.13 and we therefore have

$$\begin{aligned} \text{Tr} [\phi [T_h(A) - V] \phi]_- & \geq \int \left\{ \text{Tr} \chi_u \phi [H_0 - V_u]_- \phi \chi_u - C_\delta [h + w^2] V_u^{5/2} \Lambda_{L_1} \right. \\ & \left. - C_N V_u^{5/2} \left(\frac{h}{w L_1 V_u^{1/2}} \right)^N - C_\delta h^{-2} V_u^{1/2} \int_{B_u(2L_1)} |\nabla \otimes A|^2 + \mathcal{T}_u \right\} \frac{du}{L_1^3}. \end{aligned} \quad (6.91)$$

Estimating as around (6.17) (and choosing N sufficiently large), we get

$$\begin{aligned} \text{Tr} [\phi [T_h(A) - V] \phi]_- & \geq \int \text{Tr} \chi_u \phi [H_0 - V(u)]_- \phi \chi_u \frac{du}{L_1^3} - C_\delta h^{-2} \int_{B(2L_0)} |\nabla \otimes A|^2 \\ & - \left(C_\alpha h^\alpha + C h^2 L_1^{-2} + C L_1^2 \right) \Lambda_{L_0} + \int \mathcal{T}_u \frac{du}{L_1^3}. \end{aligned} \quad (6.92)$$

We evaluate the main term using precise semiclassics. Define $\tilde{\phi}(x) = \phi(L_0 x)$, $\tilde{V}(x) = V(L_0 x)$. Then we get by unitary scaling and applying Theorem 5.6 with the effective semiclassical parameter $\tilde{h} := h/L_0 = h^{1/2+\varepsilon_0}$ that

$$\begin{aligned}\mathcal{E}(0) &= \text{Tr} (\phi[-h^2\Delta - V]\phi)_- = \text{Tr} (\tilde{\phi}[-\tilde{h}^2\Delta - \tilde{V}]\tilde{\phi})_- \\ &= 2(2\pi\tilde{h})^{-3} \int \tilde{\phi}(x)^2 [p^2 - \tilde{V}(x)]_- dx dp + \mathcal{O}(\tilde{h}^{-1}) \\ &= 2\frac{1}{(2\pi h)^3} \int \phi(x)^2 [p^2 - V(x)]_- dx dp + \mathcal{O}(\Lambda_{L_0}\tilde{h}^2).\end{aligned}\tag{6.93}$$

By Remark 6.2

$$\begin{aligned}\int \text{Tr} \chi_u \phi[H_0 - V(u)]_- \phi \chi_u \frac{du}{L_1^3} &= \frac{2}{15\pi^2} h^{-3} \int V_-^{5/2} \phi^2 + O(L_1^2 h^{-3}) \int \phi^2 \\ &= 2\frac{1}{(2\pi h)^3} \int \phi(x)^2 [p^2 - V(x)]_- dx dp + \mathcal{O}(\Lambda_{L_0} L_1^2).\end{aligned}\tag{6.94}$$

Inserting the choices of $L_0 = h^{1/2-\varepsilon_0}$ and $L_1 = h^{1/2+\varepsilon_0}$ we get

$$\left| \mathcal{E}(0) - \int \text{Tr} \chi_u \phi[H_0 - V(u)]_- \phi \chi_u \frac{du}{L_1^3} \right| \leq C h^{1+2\varepsilon_0} \Lambda_{L_0}.\tag{6.95}$$

Finally, choosing sufficiently small δ (depending on κ) and using (6.86) and (6.95), we get (6.87). \square

6.3 Estimates on the smoothed vector field

This section is a technical preparation for the next Section 6.4. Let $A \in H^1(\mathbb{R}^3)$ be a vector field. We fix a radial function $\chi \in C_0^\infty(B(1))$ with $\int \chi = 1$ and define $\chi_r(x) = r^{-3}\chi(x/r)$ and $A_r = A * \chi_r$. We note that $\nabla \cdot A_r = 0$ on a ball $B(L)$ if $\nabla \cdot A = 0$ on $B(L+r)$.

Suppose also given ϕ' with $0 \leq \phi' \leq 1$, $\text{supp } \phi' \subset B(3L/2)$, $\phi' \equiv 1$ on $B(L)$ and $|\nabla \phi'| \leq C/L$. With this function ϕ' we define $A' = \phi' A$ and $A'_r = \phi' A_r$, then $A = A'$ and $A_r = A'_r$ on $B(L)$. The constants in the following sections may depend on χ and on the constant C in the estimate $|\nabla \phi'| \leq C/L$, but we will neglect these dependences.

Lemma 6.15. *If $r \leq L/2$, we have*

$$\|A' - A'_r\|_2^2 \leq C r^2 \int_{B(2L)} |\nabla \otimes A|^2\tag{6.96}$$

and

$$\|A' - A'_r\|_6^2 \leq C \int_{B(2L)} |\nabla \otimes A|^2.\tag{6.97}$$

Proof. We have

$$\begin{aligned}
\|A' - A'_r\|_2^2 &\leq \int_{B(3L/2)} |A - A_r|^2 = \int_{B(3L/2)} \left| \int_{B(1)} [A(x) - A(x + rz)] \chi(z) dz \right|^2 dx \\
&= \int_{B(3L/2)} \sum_{j=1}^3 \left| \int_{B(1)} \int_0^1 rz \cdot \nabla A_j(x + trz) \chi(z) dt dz \right|^2 dx \\
&\leq \frac{4\pi}{3} r^2 \int_{B(3L/2)} \sum_{j=1}^3 \int_{B(1)} \int_0^1 |z \cdot \nabla A_j(x + trz)|^2 dt dz dx,
\end{aligned} \tag{6.98}$$

by Cauchy-Schwarz. Upon changing variable in the x -integral, we obtain (6.96).

By the Sobolev inequality, we have

$$\|A' - A'_r\|_6^2 \leq C \int |\nabla \otimes (A' - A'_r)|^2 \leq C \int_{B(3L/2)} \left[|\nabla \otimes (A - A_r)|^2 + L^{-2} |A - A_r|^2 \right]. \tag{6.99}$$

In the first term we use Young's inequality, $\int_{B(3L/2)} |\nabla \otimes A_r|^2 = \int_{B(3L/2)} |\chi_r * (\nabla \otimes A)|^2 \leq \int_{B(2L)} |\nabla \otimes A|^2$, after extending the integration to \mathbb{R}^3 and using $r \leq L/2$ to insert a cutoff function $\mathbf{1}_{B(2L)}$. In the second term we use the previous calculation (6.98). \square

Lemma 6.16. *Suppose the vector field A satisfies*

$$\int_{B(2L)} A = 0. \tag{6.100}$$

Then, for all $r < L/2$ we have

$$\|A_r\|_{L^2(B(3L/2))}^2 \leq CL^2 \int_{B(2L)} |\nabla \otimes A|^2, \tag{6.101}$$

and for all multi-indices $n \in \mathbf{N}^3 \setminus \{0\}$.

$$\|\partial^n A_r\|_{L^2(B(3L/2))}^2 \leq C_n r^{2-2|n|} \int_{B(2L)} |\nabla \otimes A|^2, \tag{6.102}$$

where the constants C, C_n are independent of A, L and r .

Proof. Analogously to the proof of Lemma 6.15 we get

$$\|A_r - A\|_{L^2(B(3L/2))}^2 \leq CL^2 \int_{B(2L)} |\nabla \otimes A|^2. \tag{6.103}$$

Also, using (6.100) and the Poincaré inequality,

$$\|A_r\|_{L^2(B(3L/2))}^2 \leq \|A\|_{L^2(B(2L))}^2 \leq CL^2 \int_{B(2L)} |\nabla \otimes A|^2, \quad (6.104)$$

where, in the first step, we used $r \leq L/2$ and Young's inequality as above. This finishes the proof of (6.101).

To prove the estimate for the derivatives, for the given multi-index $n \in \mathbf{N}^3 \setminus \{0\}$, we choose $e \in \mathbf{N}^3$ with $|e| = 1$, such that $n' := n - e \in \mathbf{N}^3$, i.e., $|n| = |n'| + 1$. Then calculate

$$\begin{aligned} \|\partial^n A_r\|_{L^2(B(3L/2))}^2 &= \int_{B(3L/2)} \left| r^{-|n'|} \int_{B(1)} (\partial^{n'} \chi)(y) (\partial^e A)(x - ry) dy \right|^2 dx \\ &\leq r^{2-2|n|} \|\partial^{n'} \chi\|_2^2 \int_{B(1)} \int_{B(3L/2)} |(\partial^e A)(x - ry)|^2 dx dy \\ &\leq Cr^{2-2|n|} \int_{B(2L)} |\nabla \otimes A|^2 dx, \end{aligned} \quad (6.105)$$

where we used the assumption that $r \leq L/2$, so $B(3L/2) + B(r) \subset B(2L)$. \square

We will use the results of this section for $L = L_0 = h^{1/2-\varepsilon_0}$ where ε_0 is a small positive number. First, with the choice of $L = L_0$, by change of variable and using $r \leq L_0/2$, we get Lemma 5.7 as a consequence of Lemma 6.16. Second, we will use as an input the apriori bound (5.10), which was already proven as a result of Corollary 6.3, namely

$$h^{-2} \int_{B(2L_0)} |\nabla \otimes A|^2 \leq Ch^\alpha \Lambda_{L_0}, \quad \alpha = 1 - 3\varepsilon_0. \quad (6.106)$$

This will give bounds on various norms of $A' - A'_r$ and $\partial^n A_r$ that will be used in the next section.

6.4 Smoothing A

In this section we refine the result of Theorem 6.1 and complete the proof of Theorem 5.2 by proving (5.11). The vector potential A will not be removed as in Section 6.2, but rather replaced with A_r and this results in a smaller error. We fix three length scales $L_0 \gg L_1 \gg r$, with

$$L_0 = h^{1/2-\varepsilon_0}, \quad L_1 = h^{1/2+\varepsilon_0}, \quad r = h^{1/2+\rho}, \quad (6.107)$$

where ρ will be chosen as $\rho = C\varepsilon_0$ with a sufficiently large constant, and we assume that A satisfies (6.106). We will perform a similar analysis as in Section 6.2, in particular, we will again perform a dyadic decomposition in energy and the parameter w in the dyadic decomposition will be chosen as

$$w = h^{\alpha/2} = h^{\frac{1}{2}-\frac{3}{2}\varepsilon_0}. \quad (6.108)$$

Lemma 6.17. *For any sufficiently small $\rho > 0$ there exists a positive constant ε_0 (in fact $\varepsilon_0 = c\rho$ can be chosen where c is a universal positive constant) such that the following is satisfied. Let L_0 and r be given by (6.107), and $\phi \in C_0^\infty(B(L_0))$ with $|\partial^n \phi| \leq C_n L_0^{-|n|}$. Let V satisfy the assumptions given in Theorem 5.2. Let furthermore, A satisfy (6.106) and $\nabla \cdot A = 0$ in $B(L_0 + r)$. Then,*

$$\mathrm{Tr} [\phi[T_h(A) - V]\phi]_- \geq \mathrm{Tr} [\phi[T_h(A_r) - V]\phi]_- - Ch^{1+\varepsilon_0} \Lambda_{L_0}. \quad (6.109)$$

Since (5.10) was already proven in Corollary 6.3, Lemma 6.17 implies (5.11) and therefore finishes the proof of Theorem 5.2. The rest of this section will be devoted to the proof of Lemma 6.17.

Proof. We will use localizations as in Section 6.1 with $L = L_1$. Notice that the apriori assumption (6.14) will now be satisfied on all the small boxes $B_u(2L_1)$ with $u \in B(\frac{5}{4}L_0)$, since

$$h^{-2} \int_{B_u(2L_1)} |\nabla \otimes A|^2 \leq h^{-2} \int_{B(2L_0)} |\nabla \otimes A|^2 \leq Ch^\alpha \left(\frac{L_0}{L_1}\right)^3 \Lambda_{L_1} = Ch^{1-9\varepsilon_0} \Lambda_{L_1}, \quad (6.110)$$

where we used (6.106) and the fact that $V_u \geq c_0/2$. For the Pauli case, $T_h(A) = [\sigma \cdot (D + A)]^2$, consider

$$\begin{aligned} T_h(A) &= T_h(A_r) + \sigma(A - A_r)\sigma(D) + \sigma(D)\sigma(A - A_r) - (A - A_r) \cdot (A + A_r) \\ &= T_h(A_r) + 2D(A - A_r) - (A - A_r) \cdot (A + A_r) + h\sigma(B - B_r). \end{aligned} \quad (6.111)$$

Here we used that A and A_r are divergence free which property holds on the support of ϕ . Note that (6.111) will be used only on $\mathrm{supp} \phi$.

We denote

$$\gamma_0 := \mathbf{1}_{(-\infty, 0)}(\phi[T_h(A) - V]\phi) \quad (6.112)$$

and we collect a few apriori estimates on γ_0 .

Lemma 6.18. *With the definition (6.112) and assuming that A satisfies (6.106) and V is bounded, we get*

$$\mathrm{Tr} \gamma_0 \leq Ch^{-9\varepsilon_0/4} \Lambda_{L_0} \quad (6.113)$$

$$\mathrm{Tr} D^2 \phi \gamma_0 \phi \leq Ch^{-9\varepsilon_0/4} \Lambda_{L_0}. \quad (6.114)$$

Proof. By the variational principle and $T_h(A) \geq (D + A)^2 - |B|$,

$$\begin{aligned} \mathrm{Tr} \gamma_0 &\leq 2\mathrm{Tr}_{L^2(\mathbb{R}^3)} \mathbf{1}_{(-\infty, 0)}(\phi((D + A)^2 - |B| - V)\phi) \\ &\leq 2\mathrm{Tr}_{L^2(\mathbb{R}^3)} \mathbf{1}_{(-\infty, 0)}((D + A)^2 - (|B| + V)\mathbf{1}_{\mathrm{supp} \phi}). \end{aligned} \quad (6.115)$$

Notice that the last inequality uses the fact that we consider the strictly negative eigenvalues.

By the CLR estimate we get, since V is bounded,

$$\begin{aligned}\mathrm{Tr} \gamma_0 &\leq Ch^{-3} \int_{\mathrm{supp} \phi} (|B| + |V|)^{3/2} \leq C\Lambda_{L_0} + Ch^{-3} \int_{B(L_0)} |B|^{3/2} \\ &\leq C\Lambda_{L_0} + Ch^{-3} L_0^{3/4} \left(\int_{B(L_0)} |\nabla \otimes A|^2 \right)^{3/4} \\ &\leq C\Lambda_{L_0} + Ch^{-3} L_0^{3/4} \left(h^{2+\alpha} \Lambda_{L_0} \right)^{3/4} = Ch^{-9\varepsilon_0/4} \Lambda_{L_0}\end{aligned}$$

using (6.106) and $\alpha = 1 - 3\varepsilon_0$, which proves (6.113).

For the rest of this proof, set

$$A' = A\phi', \quad V' = V\phi', \quad (6.116)$$

where ϕ' is a cutoff function such that $\mathrm{supp} \phi' \subset B(3L_0/2)$, $\phi' \equiv 1$ on $\mathrm{supp} \phi = B(L_0)$ and $|\nabla \phi'| \leq C/L_0$. By the magnetic Lieb-Thirring inequality, Theorem 2.4, we also have,

$$\begin{aligned}0 \geq \mathrm{Tr} \phi(T_h(A') - V)\phi\gamma_0 &\geq -Ch^{-3} \int [V']^{5/2} - Ch^{-3} \left(\int |\nabla \otimes A'|^2 \right)^{3/4} \left(\int [V']^4 \right)^{1/4} \\ &\geq -C\Lambda_{L_0} - Ch^{-3} L_0^{3/4} \left(h^{2+\alpha} \Lambda_{L_0} \right)^{3/4} = -Ch^{-9\varepsilon_0/4} \Lambda_{L_0},\end{aligned} \quad (6.117)$$

using (6.106) and $\alpha = 1 - 3\varepsilon_0$. Therefore, by Schwarz and Lieb-Thirring inequalities, from (6.117) we get

$$\begin{aligned}\mathrm{Tr} D^2 \phi\gamma_0 \phi &\leq 2\mathrm{Tr} [T_h(A') + [A']^2] \phi\gamma_0 \phi \leq 2\mathrm{Tr} [V' + [A']^2] \phi\gamma_0 \phi + Ch^{-9\varepsilon_0/4} \Lambda_{L_0} \\ &\leq 2 \left(\int [V' + [A']^2]^{5/2} \right)^{2/5} \left(\int (\phi\varrho_0\phi)^{5/3} \right)^{3/5} + Ch^{-9\varepsilon_0/4} \Lambda_{L_0} \\ &\leq C \left(L_0^3 + \|A'\|_2^{1/2} \|A'\|_6^{9/2} \right)^{2/5} \left(h^{-2} \mathrm{Tr} D^2 \phi\gamma_0 \phi \right)^{3/5} + Ch^{-9\varepsilon_0/4} \Lambda_{L_0},\end{aligned} \quad (6.118)$$

where ϱ_0 is the density of γ_0 . Since $\int_{B(2L_0)} A = 0$ (see (5.7)), we have

$$\|A'\|_2^2 \leq \int_{B(2L_0)} A^2 \leq CL_0^2 \int_{B(2L_0)} |\nabla \otimes A|^2 \quad (6.119)$$

and

$$\|A'\|_6^2 \leq \int |\nabla \otimes A'|^2 \leq C \int_{B(2L_0)} [|\nabla \otimes A|^2 + L_0^{-2} |A|^2] \leq C \int_{B(2L_0)} |\nabla \otimes A|^2 \quad (6.120)$$

by Poincaré and Sobolev inequalities, thus

$$\|A'\|_2^{1/5} \|A'\|_5^{9/5} \leq CL_0^{1/5} \int_{B(2L_0)} |\nabla \otimes A|^2 \leq CL_0^{1/5} h^{2+\alpha} \Lambda_{L_0} = CL_0^{3+1/5} h^{-2\varepsilon_0}.$$

Clearly $L_0^{3+1/5}h^{-2\varepsilon_0} \ll L_0^{6/5}$, so we can continue (6.118) as

$$\mathrm{Tr} D^2\phi\gamma_0\phi \leq C\Lambda_{L_0}^{2/5} \left(\mathrm{Tr} D^2\phi\gamma_0\phi \right)^{3/5} + Ch^{-9\varepsilon_0/4}\Lambda_{L_0}$$

from which (6.114) follows since $h^{-9\varepsilon_0/4}\Lambda_{L_0} \gg 1$ if ε_0 is sufficiently small. \square

Returning to the decomposition (6.111), we first show that the effect of the quadratic term (in A) is negligible:

Lemma 6.19.

$$\left| \mathrm{Tr} (A - A_r)(A + A_r)\phi\gamma_0\phi \right| \leq C(r/L_0)^{1/10}(h^{-1}L_0^2)h^{-2-2\varepsilon_0} \int_{B(2L_0)} |\nabla \otimes A|^2. \quad (6.121)$$

In particular, assuming (6.106) and that $\rho \geq 100\varepsilon_0$, we have

$$\left| \mathrm{Tr} (A - A_r)(A + A_r)\phi\gamma_0\phi \right| \leq Ch^{\frac{1}{10}(\rho-\varepsilon_0)-7\varepsilon_0+1}\Lambda_{L_0} \leq Ch^{1+\varepsilon_0}\Lambda_{L_0}. \quad (6.122)$$

Proof. Analogously to the proof of Lemma 6.18, we use Hölder and Lieb-Thirring inequalities. The prime on the A and A_r denote localizations to $B(3L_0/2)$ as in (6.116). Then, using $\|A'\|_p \leq \|A\|_p$ and (6.119)–(6.120), we have the following estimate:

$$\begin{aligned} \left| \int (A - A_r)(A + A_r)\phi\rho_0\phi \right| &\leq \left\{ \int [(A' - A'_r)(A' + A'_r)]^{5/2} \right\}^{2/5} \left\{ \int (\phi\rho_0\phi)^{5/3} \right\}^{3/5} \\ &\leq \|A' - A'_r\|_2^{1/10} \|A' - A'_r\|_6^{9/10} \|A' + A'_r\|_2^{1/10} \|A' + A'_r\|_6^{9/10} \left\{ h^{-2} \mathrm{Tr} D^2\phi\gamma_0\phi \right\}^{3/5} \\ &\leq C \left\{ rL_0 \int_{B(2L_0)} |\nabla \otimes A|^2 \right\}^{1/10} \left\{ \int_{B(2L_0)} |\nabla \otimes A|^2 \right\}^{9/10} h^{-6/5-27\varepsilon_0/20} \Lambda_{L_0}^{3/5} \\ &\leq C(r/L_0)^{1/10}(h^{-1}L_0^2)h^{-2-2\varepsilon_0} \int_{B(2L_0)} |\nabla \otimes A|^2, \end{aligned} \quad (6.123)$$

which gives (6.121). Here we also used Lemma 6.15 with $L = L_0$ and Lemma 6.18. \square

The main problem is to estimate the current term in (6.111), i.e. the term

$$\mathrm{Tr} \left[\sigma(A - A_r)\sigma(D) + \sigma(D)\sigma(A - A_r) \right] \phi\gamma_0\phi = \mathrm{Tr} \left[2D(A - A_r) + h\sigma(B - B_r) \right] \phi\gamma_0\phi, \quad (6.124)$$

where we used that A and A_r are divergence-free on $\mathrm{supp} \phi$. We will apply localizations as in Section 6.1 with $L = L_1$ on this term. Since this is a first order operator, we can do so without localization error, using

$$\int \chi_u D\chi_u \frac{du}{L_1^3} = D \left[\frac{1}{2} \int \chi_u^2 \frac{du}{L_1^3} \right] = 0$$

for the partition of unity defined in (6.1). So we have

$$\mathrm{Tr} D(A - A_r)\phi\gamma_0\phi = \int \mathrm{Tr} \left[D(A - A_r)\eta_u\gamma_0\eta_u \right] \frac{du}{L_1^3}, \quad (6.125)$$

where we set $\eta_u := \chi_u\phi$. Similar expression holds for the terms in the first line of (6.124).

Thus, we have to estimate (see (6.116) for notation),

$$\int \mathrm{Tr} \left[(2D(A' - A'_r) + h\sigma(B' - B'_r))\eta_u\gamma_0\eta_u \right] \frac{du}{L_1^3} \quad (6.126)$$

or, equivalently,

$$\int \mathrm{Tr} \left[(\sigma(A' - A'_r)\sigma(D) + \sigma(D)\sigma(A' - A'_r))\eta_u\gamma_0\eta_u \right] \frac{du}{L_1^3}. \quad (6.127)$$

Here we have set $B' := \nabla \times A'$, $B'_r := \nabla \otimes A'_r$. We recall that, similarly to (6.45), we have

$$\int [B']^2 + \int [B'_r]^2 \leq C \int_{B(2L_0)} |\nabla \otimes A|^2.$$

We define, with V_u from (6.11),

$$H^u = D^2 - V_u, \quad \text{and} \quad P = \mathbf{1}_{(-\infty, 0]}(H^u).$$

Furthermore, we let $F_i^u, F_{>}^u, \tilde{F}_i^u, \tilde{F}_{>}^u$ be defined as in Section 6.2.1 with $W = V_u$. The parameter w entering the definition of the F 's has been fixed in (6.108) above as $w = h^{\alpha/2} = h^{\frac{1}{2} - \frac{3}{2}\varepsilon_0}$.

Lemma 6.20. *Suppose $\rho \geq 100\varepsilon_0$. Then, for any fixed $u \in B(\frac{5}{4}L_0)$ and with $\eta_u := \chi_u\phi$ we have*

$$\mathrm{Tr} \left[(\sigma(A - A_r)\sigma(D) + \sigma(D)\sigma(A - A_r))\eta_u\gamma_0\eta_u \right] \geq -Ch^{1+\varepsilon_0}\Lambda_{L_1} - Ch^{4\varepsilon_0}\mathcal{T}_u, \quad (6.128)$$

where \mathcal{T}_u was defined in (6.88).

We postpone the proof of Lemma 6.20 and first finish the proof of Lemma 6.17. Using (6.111), (6.112), the estimate (6.122) from Lemma 6.19 and (6.125), we have

$$\begin{aligned} \mathrm{Tr} [\phi[T_h(A) - V]\phi]_- &= \mathrm{Tr} [\phi[T_h(A) - V]\phi\gamma_0] \\ &\geq \mathrm{Tr} [\phi[T_h(A_r) - V]\phi\gamma_0] - Ch^{1+\varepsilon_0}\Lambda_{L_0} \\ &\quad + \int \mathrm{Tr} \left[(\sigma(A - A_r)\sigma(D) + \sigma(D)\sigma(A - A_r))\eta_u\gamma_0\eta_u \right] \frac{du}{L_1^3}. \end{aligned}$$

We now apply Lemma 6.20 and Theorem 6.14 to get

$$\begin{aligned} \mathrm{Tr} [\phi[T_h(A) - V]\phi]_- &\geq \mathrm{Tr} [\phi[T_h(A_r) - V]\phi\gamma_0] - Ch^{1+\varepsilon_0}\Lambda_{L_0} - Ch^{4\varepsilon_0} \int \mathcal{T}_u \frac{du}{L_1^3} \\ &\geq \mathrm{Tr} [\phi[T_h(A_r) - V]\phi]_- - Ch^{1+\varepsilon_0}\Lambda_{L_0}. \end{aligned} \quad (6.129)$$

This finishes the proof of Lemma 6.17. \square

Proof of Lemma 6.20. From now on we fix $u \in B(L_0 + L_1)$ and drop the u indices and superscripts for simplicity, i.e, we set $\gamma = \gamma_0$ and $\eta = \eta_u$. We rewrite the current, for each fixed u , by using (6.39), as

$$\begin{aligned}
& \text{Tr} \left[(\sigma(A - A_r)\sigma(D) + \sigma(D)\sigma(A - A_r))\eta\gamma\eta \right] \\
&= \text{Tr} \left[(\sigma(A' - A'_r)\sigma(D) + \sigma(D)\sigma(A' - A'_r))\eta(\gamma - P)\eta \right] \\
&= 2\text{Tr} [F_0^2 D(A' - A'_r)\eta(\gamma - P)\eta] \\
&\quad + 2 \sum_{i < 0} \text{Tr} [F_i^2 D(A' - A'_r)\eta(\gamma - 1)\eta] - 2 \sum_{i < 0} \text{Tr} [F_i^2 D(A' - A'_r)\eta(P - 1)\eta] \\
&\quad + 2 \sum_{0 < i \leq i_0} \text{Tr} [F_i^2 D(A' - A'_r)\eta(\gamma - P)\eta] \\
&\quad + h \sum_{i \leq i_0} \text{Tr} [F_i^2 \sigma(B' - B'_r)\eta(\gamma - P)\eta] \\
&\quad + \text{Tr} \left[F_{>}^2 (\sigma(A' - A'_r)\sigma(D) + \sigma(D)\sigma(A' - A'_r))\eta(\gamma - P)\eta \right]. \tag{6.130}
\end{aligned}$$

Note that we used formula (6.126) for all terms with $i \leq i_0$, while we used (6.127) for $i > i_0$. Notice also that the sums over negative indices can be restricted to $-i_0 \leq i < 0$, since the F_i 's vanish for larger values of $|i|$. Another important observation is that the left hand side of (6.130) is real, so it suffices to estimate the real part of each term. The estimates will be very similar to the estimates of the terms (6.48), (6.61) and (6.78) obtained during the apriori estimates in Section 6.2, but A will be replaced with $A - A_r$ and we will capitalize on the the factor $r^2 \ll L^2$ gained from the smoothing in (6.96) compared with the usual Poincaré inequality (6.30). Now we treat each term in (6.130) separately.

Step 1: The F_0 term. We write

$$\begin{aligned}
& \text{Tr} [F_0^2 D(A' - A'_r)\eta(\gamma - P)\eta] \\
&= \text{Tr} [F_0^2 D(A' - A'_r)\tilde{F}_0\eta(\gamma - P)\eta\tilde{F}_0] + \text{Tr} [F_0^2 D(A' - A'_r)\tilde{G}_0\eta(\gamma - P)\eta\tilde{F}_0]. \tag{6.131}
\end{aligned}$$

Recall that \tilde{F}_0 is slightly larger than F_0 , in particular $\tilde{F}_0 F_0 = F_0$ and $\tilde{F}_0 + \tilde{G}_0 = 1$ (see Section 6.2.1 for the precise definitions). The first term is estimated as in (6.49), with $\omega_0 = \tilde{F}_0 \eta^2 \tilde{F}_0$ and its density ϱ_0 as

$$\left| \text{Tr} [F_0^2 D(A' - A'_r)\tilde{F}_0\eta(\gamma - P)\eta\tilde{F}_0] \right| \leq C \left(\int (A' - A'_r)^2 \rho_0 \right)^{1/2} \left(\text{Tr} D^2 \omega_0 \right)^{1/2}. \tag{6.132}$$

We also used that $W = V_u$ is bounded. By the bounds on $\|\rho_0\|_\infty$ and $\text{Tr } D^2\omega_0 \leq C\text{Tr } \omega_0 \leq Cw\Lambda_{L_1}$ from (6.50) and (6.96), we have

$$\begin{aligned} |\text{Tr } [F_0^2 D(A' - A'_r) \tilde{F}_0 \eta(\gamma - P) \eta \tilde{F}_0]| &\leq C \left(h^{-3} w^2 r^2 \Lambda_{L_1} \int_{B(2L_0)} |\nabla \otimes A| \right)^{1/2} \\ &\leq Ch^{1+\rho-6\varepsilon_0} \Lambda_{L_1} \end{aligned} \quad (6.133)$$

using (6.106) and the choice of parameters (6.107), (6.108).

For the other term in (6.131), similarly to (6.51) and (6.52), we have

$$\begin{aligned} |\text{Tr } [F_0^2 D(A' - A'_r) \tilde{G}_0 \eta(\gamma - P) \eta \tilde{F}_0]| \\ \leq C \text{Tr } [D^2 \tilde{F}_0 \eta^2 \tilde{F}_0]^{1/2} \text{Tr } [F_0^2 (A' - A'_r) \tilde{G}_0^2 (A' - A'_r) F_0^2]^{1/2}. \end{aligned} \quad (6.134)$$

We apply the estimate $\text{Tr } [D^2 \tilde{F}_0 \eta^2 \tilde{F}_0] \leq Cw\Lambda_{L_1}$ as before together with the first inequality of (6.54) from the application of Lemma 6.9 to get

$$\begin{aligned} |\text{Tr } [F_0^2 D(A' - A'_r) \tilde{G}_0 \eta(\gamma - P) \eta \tilde{F}_0]| &\leq \left(Cw\Lambda_{L_1} r h^{-2} \|\nabla \otimes A\|_{L^2(B(2L_0))}^2 \right)^{1/2} \\ &\leq Ch^{1+\frac{1}{4}(2\rho-21\varepsilon_0)} \Lambda_{L_1}. \end{aligned} \quad (6.135)$$

Here we used (6.96) and that

$$\begin{aligned} \int |\nabla \otimes (A' - A'_r)|^2 &\leq \int_{B(2L_0)} |\nabla \otimes (A - A_r)|^2 + CL_0^{-2} \int_{B(3L_1/2)} |A - A_r|^2 \\ &\leq (1 + C(r/L_0)^2) \int_{B(2L_0)} |\nabla \otimes A|^2, \end{aligned} \quad (6.136)$$

to collect the A -terms. In summary, we have proved

$$\left| \text{Tr } [F_0^2 (A' - A'_r) \cdot D\eta(\gamma - P)\eta] \right| \leq Ch^{1+\varepsilon_0} \Lambda_{L_1} \leq Ch^{1+\varepsilon_0} \Lambda_{L_0} \quad (6.137)$$

assuming $\rho \geq 100\varepsilon_0$.

Step 2: $i \geq i_0 + 1$.

Lemma 6.21. *Assume that (6.106) is satisfied and that $\rho \geq 100\varepsilon_0$. Then we have*

$$\left| \text{Tr } [F_{>}^2 D(A - A_r) \eta \gamma \eta] \right| \leq 2h^{1/4} \text{Tr } [D^2 \tilde{F}_{>} \eta \gamma \eta \tilde{F}_{>}] + Ch^{5/4} \Lambda_{L_0}. \quad (6.138)$$

Proof. Recalling $\sum_{i \geq i_0+1} F_i^2 = F_{>}^2$, $F_{>} \tilde{F}_{>} = F_{>}$ and $\tilde{F}_{>} + \tilde{G}_{>} = 1$, we get

$$\begin{aligned} \text{Tr } [F_{>}^2 D(A - A_r) \eta \gamma \eta] \\ = \text{Tr } [F_{>}^2 D(A' - A'_r) \tilde{F}_{>} \eta \gamma \eta \tilde{F}_{>}] + \text{Tr } [F_{>}^2 D(A' - A'_r) \tilde{G}_{>} \eta \gamma \eta \tilde{F}_{>}]. \end{aligned} \quad (6.139)$$

The first term we estimate as

$$\left| \text{Tr} [F_{>}^2 D(A' - A'_r) \tilde{F}_{>} \eta \gamma \eta \tilde{F}_{>}] \right| \leq \left(\text{Tr} [F_{>}^4 D^2 \tilde{F}_{>} \eta \gamma \eta \tilde{F}_{>}] \text{Tr} [(A' - A'_r)^2 \tilde{F}_{>} \eta \gamma \eta \tilde{F}_{>}] \right)^{1/2}. \quad (6.140)$$

In the last factor we apply Hölder, Sobolev and Lieb-Thirring inequalities similarly to (6.123) to get

$$\begin{aligned} \text{Tr} [(A' - A'_r)^2 \tilde{F}_{>} \eta \gamma \eta \tilde{F}_{>}] &\leq \|A' - A'_r\|_2^{1/5} \|A' - A'_r\|_6^{9/5} \left(h^{-2} \text{Tr} [D^2 \tilde{F}_{>} \eta \gamma \eta \tilde{F}_{>}] \right)^{3/5} \\ &\leq r^{1/5} h^{-6/5} \int_{B(2L_1)} |\nabla \otimes A|^2 \left(\text{Tr} [D^2 \tilde{F}_{>} \eta \gamma \eta \tilde{F}_{>}] \right)^{3/5}. \end{aligned} \quad (6.141)$$

Inserting this into (6.140), using $\tilde{F}_{>}^2 \leq 1$, we find

$$\begin{aligned} \left| \text{Tr} [F_{>}^2 D(A' - A'_r) \tilde{F}_{>} \eta \gamma \eta \tilde{F}_{>}] \right| &\leq r^{1/10} h^{-3/5} \left(\int_{B(2L_1)} |\nabla \otimes A|^2 \right)^{1/2} \left(\text{Tr} [D^2 \tilde{F}_{>} \eta \gamma \eta \tilde{F}_{>}] \right)^{4/5} \\ &= \tau^{5/4} \text{Tr} [D^2 \tilde{F}_{>} \eta \gamma \eta \tilde{F}_{>}] + \tau^{-5} r^{1/2} h^{-3} \left(\int_{B(2L_1)} |\nabla \otimes A|^2 \right)^{5/2} \\ &\leq \tau^{5/4} \text{Tr} [D^2 \tilde{F}_{>} \eta \gamma \eta \tilde{F}_{>}] + \tau^{-5} (h^{5+\rho-24\varepsilon_0})^{1/2} \Lambda_{L_0} \end{aligned} \quad (6.142)$$

for any $\tau > 0$, and where we used (6.106) to get the last estimate.

We now consider the second term in (6.139). By a Cauchy-Schwarz inequality and by applying Lemma 6.9 (recall (6.33)) similarly as in (6.134)–(6.136), we find

$$\begin{aligned} \left| \text{Tr} [F_{>}^2 D(A' - A'_r) \tilde{G}_{>} \eta \gamma \eta \tilde{F}_{>}] \right| &\leq \left(\text{Tr} [D^2 \tilde{F}_{>} (\eta \gamma \eta)^2 \tilde{F}_{>}] \text{Tr} [F_{>}^2 (A' - A'_r) \tilde{G}_{>}^2 (A' - A'_r) F_{>}^2] \right)^{1/2} \\ &\leq \tau \text{Tr} [D^2 \tilde{F}_{>} \eta \gamma \eta \tilde{F}_{>}] + \tau^{-1} h^{-2} r \int_{B(2L_1)} |\nabla \otimes A|^2 \\ &\leq \tau \text{Tr} [D^2 \tilde{F}_{>} \eta \gamma \eta \tilde{F}_{>}] + \tau^{-1} h^{\frac{3}{2}+\rho-3\varepsilon_0} \Lambda_{L_0}, \end{aligned} \quad (6.143)$$

where we used (6.106) to get the last estimate.

Combining (6.142) and (6.143), we get (6.138) by choosing $\tau = h^{1/4}$. \square

Step 3: $|i| \leq i_0 + 1$.

Lemma 6.22. *If $\rho > 100\varepsilon_0$,*

$$\begin{aligned}
& \Re \left\{ 2 \sum_{i < 0} \text{Tr} [F_i^2 D(A' - A'_r) \eta (\gamma - 1) \eta] - 2 \sum_{i < 0} \text{Tr} [F_i^2 D(A' - A'_r) \eta (P - 1) \eta] \right. \\
& \quad + 2 \sum_{0 < i \leq i_0} \text{Tr} [F_i^2 D(A' - A'_r) \eta (\gamma - P) \eta] \\
& \quad \left. + h \sum_{i \leq i_0} \text{Tr} [F_i^2 \sigma(B' - B'_r) \eta (\gamma - P) \eta] \right\} \\
& \geq -Ch^{4\varepsilon_0} \sum_{i \leq i_0} 2^i w \text{Tr} [D^2 F_i^2 \eta \gamma \eta] \\
& \quad - Ch^{4\varepsilon_0} \sum_{0 > i \geq i_0} 2^{|i|} w \text{Tr} [D^2 F_i^2 \eta (1 - \gamma) \eta] - Ch^{1+\varepsilon_0} \Lambda_{L_0}. \tag{6.144}
\end{aligned}$$

Proof. Consider $0 < i \leq i_0$. We write

$$\text{Tr} [F_i^2 D(A' - A'_r) \eta \gamma \eta] = \text{Tr} [F_i^2 D(A' - A'_r) \tilde{F}_i \eta \gamma \eta] + \text{Tr} [F_i^2 D(A' - A'_r) \tilde{G}_i \eta \gamma \eta], \tag{6.145}$$

using $\tilde{F}_i + \tilde{G}_i \equiv 1$. We can estimate the first term, using $F_i \tilde{F}_i = F_i$, as,

$$\begin{aligned}
\left| \text{Tr} [F_i^2 D(A' - A'_r) \tilde{F}_i \eta \gamma \eta] \right| & \leq \left\{ \text{Tr} [F_i^4 D^2 \tilde{F}_i \eta \gamma \eta \tilde{F}_i] \right\}^{1/2} \left\{ \text{Tr} [(A' - A'_r)^2 \tilde{F}_i \eta \gamma \eta \tilde{F}_i] \right\}^{1/2} \\
& \leq h^{4\varepsilon_0} 2^i w \text{Tr} [D^2 F_i^2 \eta \gamma \eta] + h^{-4\varepsilon_0} 2^{-i} w^{-1} \text{Tr} [(A' - A'_r)^2 \tilde{F}_i^2] \\
& \leq h^{4\varepsilon_0} 2^i w \text{Tr} [D^2 F_i^2 \eta \gamma \eta] + Ch^{-4\varepsilon_0} h^{-3} r^2 \int_{B(2L_0)} |\nabla \otimes A|^2 \\
& \leq h^{4\varepsilon_0} 2^i w \text{Tr} [D^2 F_i^2 \eta \gamma \eta] + Ch^{1+2\rho-7\varepsilon_0} \Lambda_{L_0}, \tag{6.146}
\end{aligned}$$

where we used (6.80) and (6.96) in the third inequality. Then we used (6.106) and the choice of parameters (6.107) to finish the estimate. This is in agreement with the desired estimate if $\rho > 100\varepsilon_0$ (since the number of terms i_0 in the sum is only logarithmic in h).

The remaining term in (6.145) is estimated using Lemma 6.9 and that $\|\nabla f_i\|_1 \leq CW \leq C$:

$$\begin{aligned}
\left| \text{Tr} [F_i D F_i (A' - A'_r) \tilde{G}_i \eta \gamma \eta] \right| & \leq \left\{ \text{Tr} [F_i^2 D^2 \eta \gamma \eta] \right\}^{1/2} \left\{ \text{Tr} [\tilde{G}_i (A' - A'_r) F_i^2 (A' - A'_r) \tilde{G}_i \eta \gamma \eta] \right\}^{1/2} \\
& \leq h^{4\varepsilon_0} \cdot 2^i w \text{Tr} [F_i^2 D^2 \eta \gamma \eta] + Ch^{-4\varepsilon_0} \frac{r h^{-2}}{2^i w} \|\nabla \otimes A\|_{L^2(B(2L_0))}^2 \\
& \leq h^{4\varepsilon_0} \cdot 2^i w \text{Tr} [F_i^2 D^2 \eta \gamma \eta] + Ch^{1+\rho-6\varepsilon_0} \Lambda_{L_0}. \tag{6.147}
\end{aligned}$$

This is in agreement with (6.144) if $\rho > 100\varepsilon_0$.

We also estimate the corresponding term with P .

$$\begin{aligned}
\left| \text{Tr} [F_i^2 D(A' - A'_r) \eta P \eta] \right| & \leq \left\{ \text{Tr} [F_i^2 D^2 \eta P \eta] \text{Tr} [P \eta (A' - A'_r) F_i^2 (A' - A'_r) \eta P] \right\}^{1/2} \\
& = \|D F_i \eta P\|_{HS} \left\{ \text{Tr} [P \eta (A' - A'_r) F_i^2 (A' - A'_r) \eta P] \right\}^{1/2}. \tag{6.148}
\end{aligned}$$

Using (6.84) and that $(h/wL) = h^{\varepsilon_0/2}$, the first factor can be made smaller than an arbitrarily large power of h , while the second one is bounded by $\Lambda_{L_1}^{1/2} \|A' - A'_r\|_2$, which is not bigger than a fixed positive power of h . So this term is negligible. The similar terms for negative indices i are estimated in the same manner with only notational changes.

Also the $\sigma(B' - B'_r)$ terms are readily controlled. We leave this part to the reader. \square

We can now finish the proof of Lemma 6.20. We combine (6.130) with (6.137) and the results of Lemma 6.21 and 6.22. This finishes the proof of Lemma 6.20. \square

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